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AOC Parties Technical Working Group Meeting No. 14 A Potential Approach Being Considered by the Navy: Simplified 3-D LNAPL Numerical Modeling

AOC SOW Section 6 and Section 7
Red Hill Bulk Fuel Storage Facility

March 4, 2019 0800–1200 HST

Agenda

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0800 – 0815	Introductions
0815 – 0830	Opening Comments
0830 – 0845	Navy's Modeling Objectives and Feedback on 2-D Modeling Approach
0845 – 0915	Approach and Formulation for Simplified Modeling
0915 – 0945	Verification of Simplified Approach ***This is not an analysis specific to Red Hill, and used for comparative LNAPL (gasoline) simulations between the Simplified LNAPL Model and UTCHEM***
0945 – 1000	Break
1000 – 1045	Simulation of LNAPL Migration in the Vadose Zone and on the Water Table ***This is not an analysis specific to Red Hill, and used for LNAPL (gasoline) simulations using the Simplified LNAPL Model to understand migration behavior for various parameter and combination values***
1045 – 1100	Key Parameters for LNAPL Migration Evaluations
1100 – 1130	Demonstration of Simulation Approach at Red Hill ***This is for demonstration purposes only, and future efforts will be aligned with the Navy's modeling objectives.***
1130 – 1140	Potential Path Forward
1140 – 1200	Open Discussion

* UTCHEM – A 3-D chemical flux simulator prepared UT (2000)

Purpose of AOC Parties TWG Meeting No. 14

- Brief overview of progress: where we were, where we've been, and where we're going
- Provide technical feedback to the Regulatory Agencies on the 2-D LNAPL modeling approach proposed during February 13's Technical Working Group meeting
- Present to the Regulatory Agencies another potential approach to LNAPL modeling that the Navy is currently considering
- Solicit feedback and also gain consensus from the Regulatory Agencies that this approach has merit and is worth pursuing
- Describe constraints moving forward in order to achieve alignment
  - Limited timeframe
  - Alignment on parameters and values
  - Alignment on LNAPL scenarios
  - Alignment on usability of the model (e.g. uncertainty, decision process, etc.)

Progress Thus Far and Where We Are Now: LNAPL Modeling

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- During the 2015–2016 AOC SOW Sections 6/7 Scoping Meetings, it was agreed upon by the AOC Parties that numerical LNAPL modeling is not be performed primarily due to:
  - Collective agreement to not drill borings within the Facility for protection of the aquifer
  - High degree of uncertainty (and therefore low confidence in usability of the model) associated with high heterogeneity of the geologic system and a limited dataset

- It was agreed upon by the AOC Parties that a “best estimate” would be employed to reasonably bound LNAPL impacts with conservative assumptions (i.e. LNAPL holding capacity estimate as documented in the interim report)

- The LNAPL holding capacity approach in the July 2018 Interim Report was intended to address two conditions: potential small chronic releases and larger, acute releases

- Navy received the Regulatory Agencies’ “Top 10 Comments” in August 2018, and requested an extension in September 2018 that assumed a limited LNAPL evaluation (not numerical modeling as stated in our request letter and consistent with prior agreement)

Progress Thus Far and Where We Are Now: LNAPL Modeling

- Regulatory Agencies have recently expressed a strong desire to conduct numerical LNAPL modeling in order to help understand: (1) the extent of LNAPL migration due to various source terms, and (2) the timing related to how quickly LNAPL may migrate in the environment

- During the last technical working group meeting on February 13, the Regulatory Agencies recommended a 2-D LNAPL modeling approach

- In pursuit of deliverable acceptability by the Regulatory Agencies, technical defensibility, and reasonable conservatism, the Navy is currently evaluating another potential approach to LNAPL evaluation – simplified 3-D modeling approach

Progress Thus Far and Where We Are Now: LNAPL Modeling

- The February 13 technical working group meeting was useful in that it outlined key elements of an approach to LNAPL numerical modeling that would be acceptable to the Regulatory Agencies

- The Navy has considered this recommended approach, and is currently considering another potential approach to meet the Regulatory Agencies' goals as described in the February 13 presentation. **This potential approach is for evaluation and solicitation of feedback, and is not being formally proposed at this time.**
  - The approach is similar to the approach outlined by the Regulatory Agencies in that it tests the impact of various potential LNAPL releases conceptually to understand behavior and bracket impacts
  - The approach is different in that the limitations of 2-D are eliminated
  - The approach is different in that the equations solved are simplified with appropriate assumptions instead of dimensionality

Red Hill AOC SOW
Contaminant Fate and Transport Priorities

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- Protect drinking water receptors and groundwater resource
- Inform future actions regarding:
  - Infrastructure improvements (TUA)
  - Sentinel well network placement
  - Release response

Navy's Groundwater Modeling Objective

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The objective of groundwater modeling is to help ascertain potential risk to water supply wells as a result of a potential range of releases from the Red Hill Bulk Fuel Storage Facility under a range of reasonably conservative pumping conditions within the model domain. The results of this modeling effort will then be used to:

1. Inform decisions related to the Tank Upgrade Alternatives (TUA), and
2. Inform decisions related to potential remedial alternatives

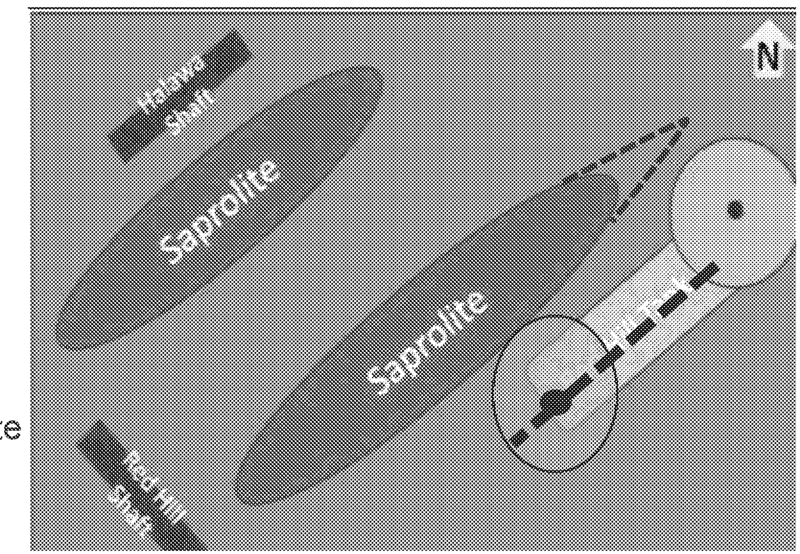
Pursuant to the Administrative Order on Consent Statement of Work Section 6, Investigation & Remediation of Releases, and Section 7, Groundwater Protection and Evaluation

Navy's Modeling Objective for the Interim Report

- The holding capacity analysis was based on observed NSZD rates as well as thermal profiling and was designed to inform AOC Parties of the following:
  1) the size of a chronic (small) release that would not impact groundwater
     - A Monte Carlo analysis was conducted in an effort to describe the uncertainty which is a conservative approach.
  2) the size of an acute release that would not impact groundwater.
- The holding capacity analysis was not designed to inform AOC Parties as to the extent and timing associated with various LNAPL release scenarios, since numerical LNAPL modeling was originally deemed inappropriate by the AOC Parties.

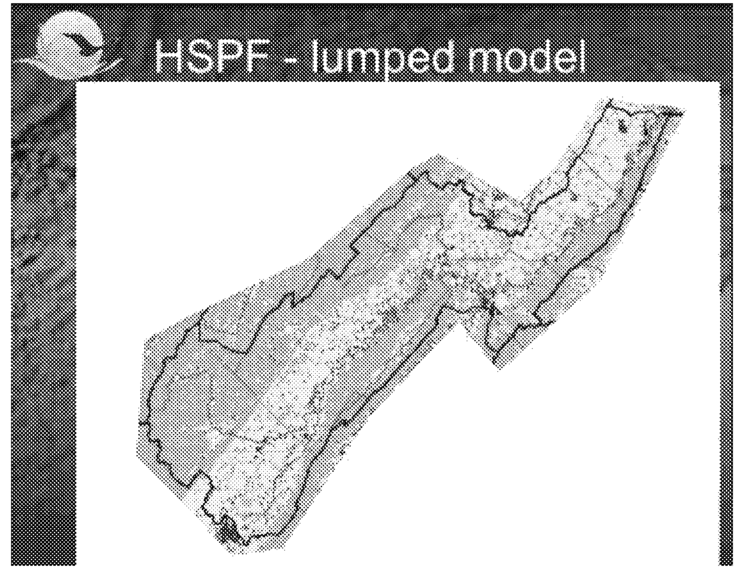
Navy's Proposed LNAPL Modeling Objectives

- Update the holding capacity analysis based on new geologic information
- Conduct new LNAPL modeling as an additional effort by the Navy using a simplified 3-D model to evaluate various potential LNAPL release scenarios (as part of a bounding effort) at Red Hill as follows:
  - Evaluate a range of release rates including:
    - Small Chronic Release
    - Intermediate Release (2014 Tank 5 Release)
    - Large Release
    - Catastrophic Release (Tunnel Impact)
  - Evaluate potential LNAPL migration with regard to
    - Red Hill Shaft (release at lower tanks)
    - Halawa Shaft (release at higher tanks)
      - Considering two conceptualizations of the saprolite
  - Consider pre-existing residual LNAPL saturation
  - Compare 3-D and lumped-model holding capacities
  - Provide source terms for GW F&T modeling
  - The LNAPL effort along with the groundwater modeling effort will be used to:
    1. Inform decisions related to the TUA,
    2. Inform decisions related to placement of additional monitoring/sentinel wells, and
    3. Inform decisions related to potential remedial alternatives



But first …

- Don't knock lumped models
  - They may not be suitable for all cases, BUT
  - They have proved useful for decades and continue to do so
    - HSPF and PRMS lumped parameter models for hydrological studies
  - Application for current analyses
    - Determine holding capacity
    - Compare results with transport model using similar parameters and assumptions
    - Explore uncertainty using Monte Carlo simulations



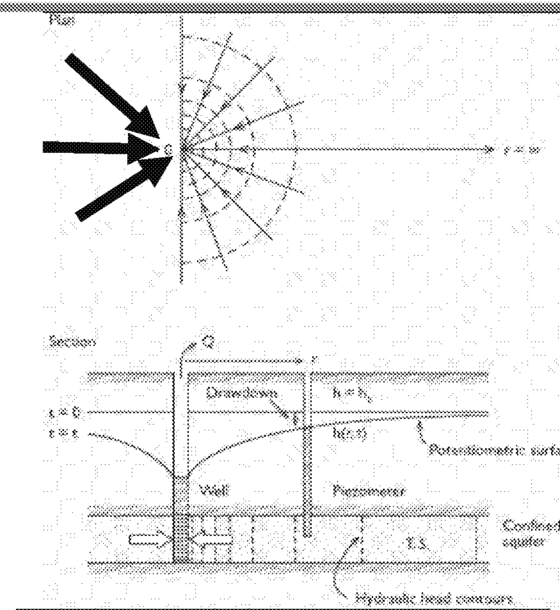
Chesapeake Bay Program Modeling HSPF - lumped model

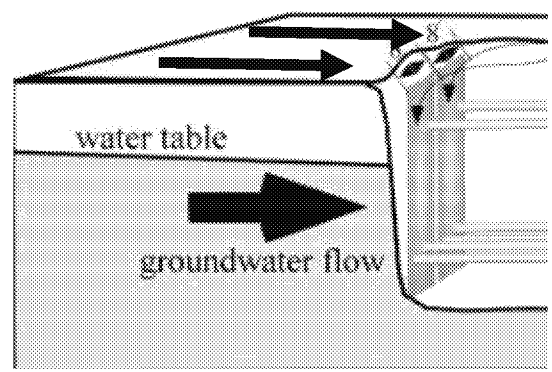
HSPF: Bicknell, B.R., Imhoff, J.C., Kittle, J.L., Jr., Donigian, A.S., Jr., and Johanson, R.C., 1997, Hydrological Simulation Program--Fortran: User's manual for version 11: U.S. Environmental Protection Agency, National Exposure Research Laboratory, Athens, Ga., EPA/600/R-97/080, 755 p.

PRMS: Markstrom, S.L., Regan, R.S., Hay, L.E., Viger, R.J., Webb, R.M.T., Payn, R.A., and LaFontaine, J.H., 2015, PRMS-IV, the precipitation-runoff modeling system, version 4: U.S. Geological Survey Techniques and Methods, book 6, chap. B7, 158 p., https://dx.doi.org/10.3133/tm6B7.

And also …

- Anything 2-D can do, 3-D can do better
  - Except speed – if the same equation set is being solved
  - 3-D can always exactly mimic 2-D so it can be at least as good
  - 2-D (vertical and horizontal) models have their roles ***and assumptions***
  - Point sources / sinks can lead to unrealistic results with 2-D cross-sectional models (violates 2-D assumptions)
  - Vertically integrated modeling codes (OILENS model in HSSM) required for areal 2-D simulations – on water table



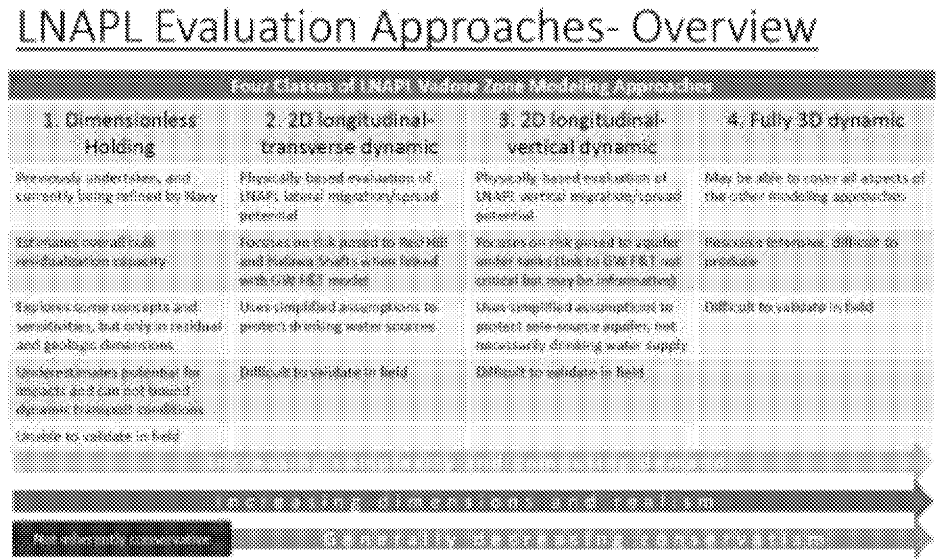


OILENS: Model for spreading of LNAPL above the water table in HSSM.

HSSM: R.J., Charbeneau, J.W. Weaver, and B.K. Lien 1995. The Hydrocarbon Spill Screening Model, EPA/600/R-94/039b.

Issues with Agencies' LNAPL Evaluation Approaches – Overview

- Any model will be difficult/impossible to validate (no LNAPL in wells to calibrate against but do have NSZD/GW chemistry data to help bound things).
- Certain fully dynamic models such as UTCHEM may not properly work for the conditions being considered at Red Hill.
- Two-dimensional analyses do not take into account effects of the third dimension, which can be significant when the required assumptions are not satisfied.



LNAPL Evaluation Approaches- Overview

Four Classes of LNAPL Vadose Zone Modeling Approaches			
1. Dimensionless Holding	2. 2D longitudinal-transverse dynamic	3. 2D longitudinal-vertical dynamic	4. Fully 3D dynamic
Previously undertaken, and currently being refined by Navy	Physically based evaluation of LNAPL lateral migration/spread potential	Physically based evaluation of LNAPL vertical migration/spread potential	May be able to cover all aspects of the other modeling approaches
Estimates overall bulk residualization capacity	Focuses on risk posed to Red Hill and Halawa Shafts when linked with GW F&T model	Focuses on risk posed to aquifer under tanks (link to GW F&T not critical but may be informative)	Resource intensive, difficult to produce
Explores some concepts and sensitivities, but only in residual and geologic dimensions	Uses simplified assumptions to protect drinking water sources	Uses simplified assumptions to protect sole-source aquifer, not necessarily drinking water supply	Difficult to validate in field
Underestimates potential for impacts and can not bound dynamic transport conditions	Difficult to validate in field	Difficult to validate in field	
Unable to validate in field			

*From February 13 regulatory AOC Technical Working Group presentation

Two-dimensional vertical slice assumption is violated when source is not a line perpendicular to flow directions.

Example simulation demonstrates 4 times quicker movement of LNAPL with a 2-D vertical slice than for a three-dimensional counterpart simulation.

Two dimensional aerial slice neglects vertical flow. Example simulations indicate that even with extreme anisotropy and extreme slope of the geologic formation, there is vertical movement through the formation.

Example simulations demonstrate 5 to 15 times quicker movement of LNAPL along a 2-D aerial slice, than for a three dimensional counterpart simulation where LNAPL has to pass vertically through 100 feet of soil.

Due to these factors, the Navy is considering a simplified 3-D LNAPL modeling approach over the 2-D LNAPL modeling approach proposed by the Regulatory Agencies

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Approach and Formulation for Simplified Modeling

Standard Approach – Multiphase Modeling

- Multiphase flow modeling is complex and computationally intensive
  - Solves for multiple equations per computational cell
  - Extremely nonlinear nature of the interactions between the phases
  - Extremely nonlinear constitutive relationships (multiphase retention and relative permeability functions)
  - Air flow solution – which determines flow rates of air – causes a lot of the difficulty
- Simplifying assumptions that are made to enable required analyses include
  - Coarse gridding
  - Reduced (1-D or 2-D) dimensionality
  - Simplified geometries
  - Small areal extents
  - Smoothed parameterization
  - Limited evaluations
- Often these assumptions for certain multiphase models render results unusable or unreliable

- ***Assumptions for reducing the equation set may be more applicable and practical***

Simplified Modeling Approach

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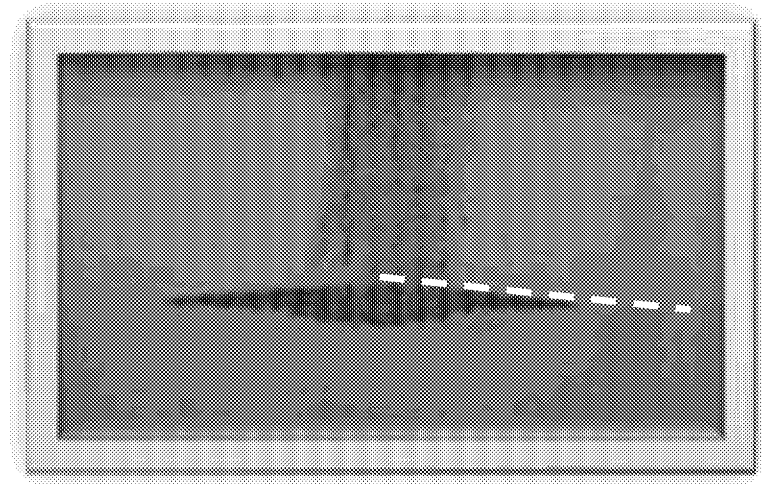
- Reduce governing multiphase flow equations using appropriate approximations to simplify and speed up computations
  - Solve only one (LNAPL-phase) equation for evaluating LNAPL flow in the vadose zone and along the water table
- Why is it important and useful
  - Can accommodate larger domain, finer grid, three-dimensional representation and structural complexity that may be difficult or impossible to represent and solve at a complex contaminated site with a multi-phase flow model
    - Significantly alleviates computational burden
      - Depending on code used, the solution can often fail even for very simple conditions
      - Model that runs quickly can test many alternative conceptualizations and parameter distributions and ranges to bracket likely behavior
    - Reduces parameterization burden (only needed for LNAPL phase)
      - Parameterization of unsaturated and saturated zones at a site is difficult
      - Parameterization of multi-phase flow is difficult
  - Readily adaptable to open source, public domain codes such as MODFLOW-USG, or other unsaturated single-phase flow codes
  - Can bracket the impacts of the assumptions used to neglect water phase flow

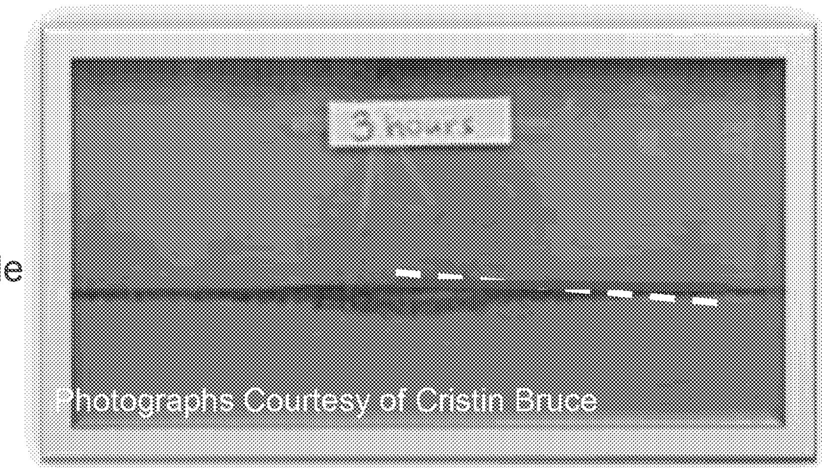
Simplified Modeling Approach Assumptions

- Assume air phase to instantly equilibrate to movement of liquids
  - Valid for unsaturated zone flow (this is not a petroleum reservoir)
  - Validated for flow of water in the vadose zone using Richards Equation
  - Reduces air flow equation
- Assume state of water to remain unchanged by neglecting water flow dynamics and water redistribution
  - Appropriate at residual water saturations above capillary fringe
  - Neglects depression of water table by pressure of overlying LNAPL – lateral LNAPL spread will be larger than computed so impact is conservative
  - Can bound impacts of LNAPL in capillary fringe and depression of water table
  - Reduces water flow equation
- Solve LNAPL flow equation only
  - Simplify constitutive relationships such that air-filled pore space is the porosity available for LNAPL flow – reduces 3-phase relations to standard 2-phase air-LNAPL equations readily solved by available unsaturated zone flow codes.

Estimated Impact of Proposed Approach

- Reducing flow equation of air:
  - Richards equation approximation of neglecting air phase dynamics is appropriate for unsaturated zone flow calculations and is commonly applied in practice – no impact
- Reducing flow equation of water:
  - The unsaturated zone already has residual LNAPL in certain areas, and thus conditions are not pristine where interfacial tension changes between air-water interface are now mediated through a LNAPL interface (which usually causes an initial flush of water preceding the LNAPL front) – no impact for current objectives
  - Unsaturated zone typically has water at residual saturation conditions, and thus impact of water displacement due to presence of LNAPL will be negligible – small impact for current objectives
  - Near water table, and at water table, water will be depressed by pressure of overlying LNAPL and that is neglected – lateral LNAPL spread will be smaller than computed (impact is conservative)





Photographs Courtesy of Cristin Bruce

Estimated Impact of Proposed Approach (continued)

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- Solving only flow equation of LNAPL:
  - Simulates LNAPL dynamics including capillarity and permeability – provides a detailed analysis of LNAPL flow
    - Hydraulic conductivity scaling using density and viscosity ratios provides LNAPL conductivity
    - Moisture retention curves can be scaled to represent retention and relative permeability with respect to LNAPL
  - Porosity represents air and LNAPL filled pores to convert 3-phase retention curves to 2-phase curves – accounts for water filling part of the pore space, which is most critical within capillary fringe
  - Significantly faster runtimes than solving 3-phase flow equations – less chance of failure of complex coupled solutions and greater ability to represent complex geometries
    - Simulation run times for all models discussed here is between 10 and 30 minutes using the simplified LNAPL modeling approach
    - Simulation run times were over 9 hours using UTCHEM ***(20 to 50 times longer)***
  - Can use MODFLOW-USG Richards equation capability – control over simulator and required modifications. Availability of pre- and post-processing tools for faster data manipulation

Formulation and Governing Equations

- Please request details if interested – manuscript for Journal article is under preparation

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Verification of Simplified Approach Against Multiphase Modeling

Purpose/Qualifying Points

- This is a non-Red Hill analysis for comparative LNAPL (gasoline) simulations between the Simplified LNAPL Model and UTCHEM
- The behavior of gasoline in this model should not be considered like a jet fuel, since viscosities are significantly different
- The simulation objective was comparison of models and not the value of any specific parameter

Test Simulations with MODFLOW-USG and UTCHEM

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- LNAPL (gasoline) migration through a horizontally bedded unsaturated soil to a horizontal water table
- LNAPL (gasoline) migration through a sloping bedded unsaturated soil

- ***But first … some parameters for gasoline***
  - *Gasoline was initially used for the comparative analysis, and some jet fuel simulations will be described later*

Some Parameters for LNAPL (gasoline) and Water

- Density of water = 1 = ρ_w
- Density of LNAPL = 0.73 = ρ_n
- Viscosity of water = 0.89 cP = μ_w
- Viscosity of gasoline = 0.5 cP = μ_n

$$K_n = \frac{\rho_n}{\mu_n}\frac{\mu_w}{\rho_w}K_w = 1.3K_w$$

So, for K_w = 5,000 ft/d; K_n = 6,500 ft/d

  - K_w = Hydraulic conductivity
  - K_n = Flow conductivity to NAPL

- Porosity = 0.1
- Water residual saturation = 0.3 = S_{wr}
- LNAPL residual saturation = 0.14 (= 0.2 in modified pore space) = S_{nr}
- Continuous LNAPL release of 30,000 gal/d (4,010 cu-ft/d) over a 100 ft x 100 ft area beginning at time = 0.

Some More Parameters for LNAPL (gasoline) and Water

- Interfacial tension for air water = 72.7 dynes/cm = 0.0727 N/m = σ_{aw}
- Interfacial tension for air LNAPL = 21 dynes/cm = 0.021 N/m = σ_{an}
- Interfacial tension for LNAPL water = 52 dynes/cm = 0.052 N/m = σ_{nw}

$$\beta_{nw} = \frac{\sigma_{aw}}{\sigma_{nw}} = 1.4 \qquad \beta_{an} = \frac{\sigma_{aw}}{\sigma_{an}} = 3.46$$

- van Genuchten Alpha for air-water system = 0.44 (1/ft)
- van Genuchten Beta = 2.68
- Brooks Corey "n" = 4.19 (generally related to van Genuchten parameters as):

$$n = 1 + \frac{2\beta}{(\beta - 1)}$$

- Scaled Alpha for LNAPL-water system = 0.44*1.4 = 0.62 (1/ft)
- Scaled Alpha for air-LNAPL system = 0.44*3.46 = 1.52 (1/ft)

Revised Parameters for LNAPL (gasoline) and Water on UTCHEM Runs

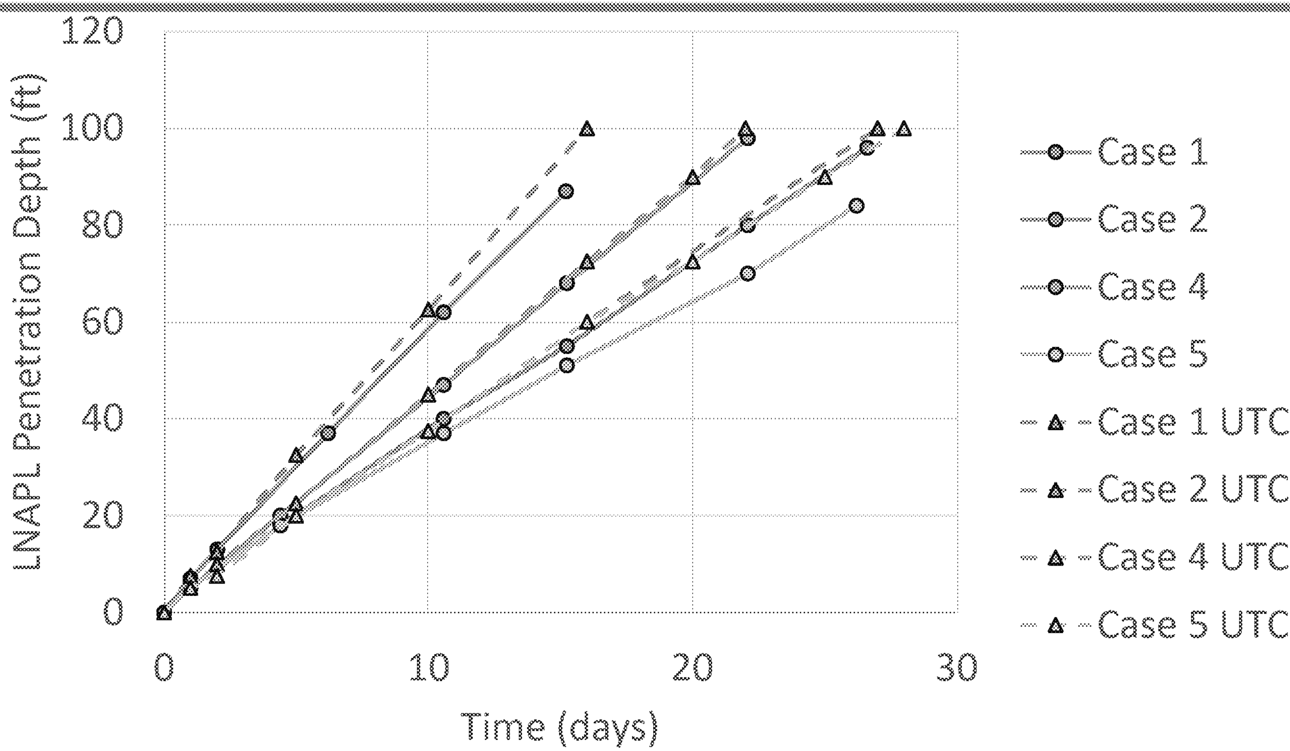
- van Genuchten Alpha for air-water system = 8.28 (1/ft)
- van Genuchten Beta = 1.59
- Brooks Corey "n" = 6.4
- Scaled Alpha for LNAPL-water system = 8.28 *1.4 = 11.6 (1/ft)
- Scaled Alpha for air-LNAPL system = 8.28 *3.46 = 28.6 (1/ft)
- Residual LNAPL saturation = 0.2 in original porosity
  - = 0.28 in modified porosity
  - P-kr-s curve: van Genuchten Beta of 2 fits original curve better when residual saturation is zero
- Release rate = 50 m^3/d = 1,766 cu-ft/d

➢ UTCHEM does not run under many Red Hill conditions

UTCHEM Comparison Simulation Test Cases

			Kh	Kz	A-N van G alpha	Brooks Corey exponent
Example	Source (ft^3/d)	Slope	(ft/d)	(ft/d)	(1/ft)	
Case 1	1,766 continuous	0%	*5,000*	*5,000*	28.6	6.4
Case 2	1,766 continuous	0%	*5*	*5*	28.6	6.4
Case 3	1,766 ***for 10 days***	0%	5	5	28.6	6.4
Case 4	1,766 continuous	0%	*50*	*50*	28.6	6.4
Case 5	1,766 continuous	0%	*50*	*5*	28.6	6.4
Case 6	1,766 continuous	*3%*	***5,000***	***5***	28.6	2.0

Comparison of Single-Phase Model with UTCHEM Results



Case 3:

For both simulations, LNAPL did not reach the water table.

Redistribution of LNAPL to a depth of 60 feet by 200 days with single-phase model

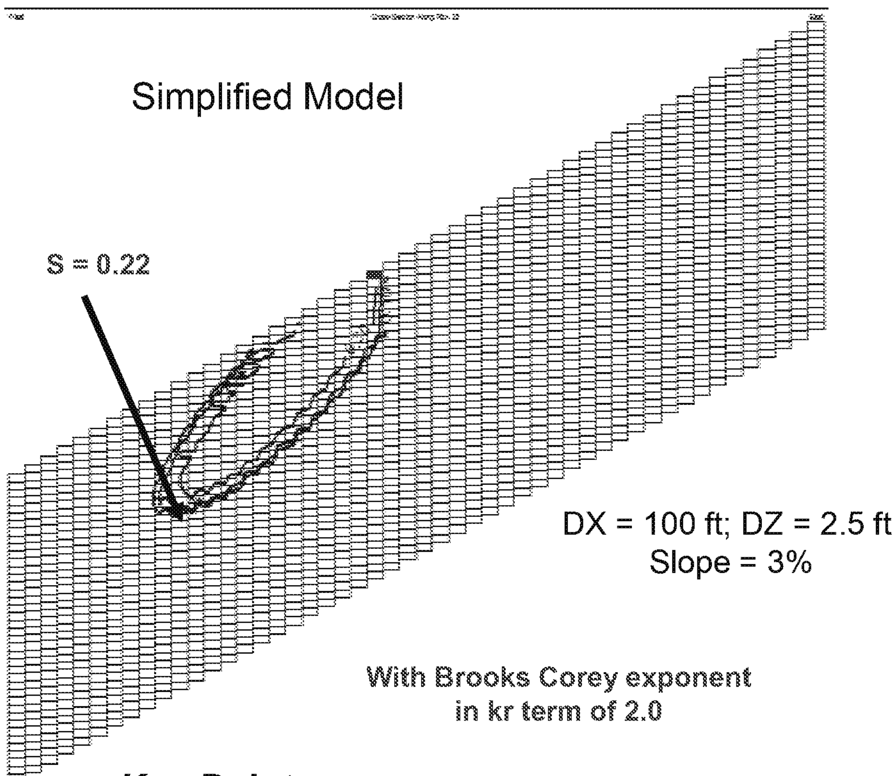
Redistribution of LNAPL to a depth of 62.5 feet by 200 days with UTCHEM

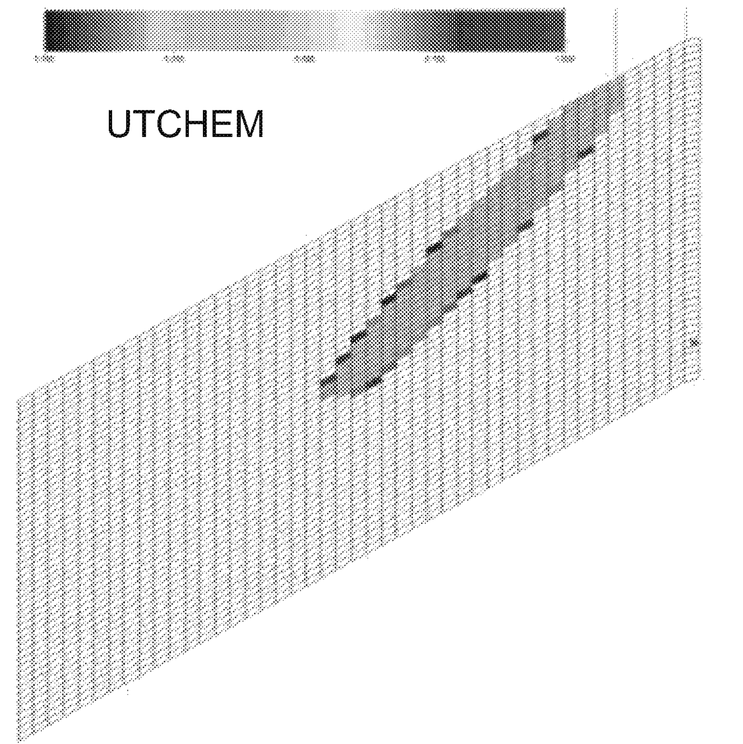
Key Points:

- Comparison between UTCHEM and single phase model results is good for all simulation cases
- Case 5 of UTCHEM includes anisotropy. It is not clear how the Leverett scaling ($\sqrt{K/\phi}$) is applied to the retention curves under anisotropic conditions in UTCHEM.
- Different multiphase codes adapt different scaling and 3-phase constitutive relationships – UTCHEM has a Leverett scaling which is directional depending on K
- Differences can also be attributed to differences in numerical schemes (upstream implicit versus mid-point IMPES – Implicit Pressure, Explicit Saturation)

Comparison of Single-Phase Model with UTCHEM Results for Case 6

UTCHEM scales the retention function depending on the K-value but it is not clear how that is done when there is anisotropy in the K-value





Key Points:

- Comparison between UTCHEM and single-phase model is good (scale of two graphs is not the same)
- Strict apples-to-apples comparison could not be made due to Leverett scaling in UTCHEM
- Multiphase codes also have their differences in numerical schemes, averaging methods, spatial discretization, and scaling of multiphase constitutive relations, causing differences in results

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Simulation of LNAPL (Gasoline) Migration in the Vadose Zone and on the Water Table for Various Geologic and Fluid Conditions

Purpose/Qualifying Points

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- This is a non-Red Hill analysis of LNAPL (gasoline) simulations using the Simplified LNAPL Model to understand migration behavior for various parameter and combination values
- The behavior of gasoline in this model should not be considered like a jet fuel, since viscosities are significantly different
- The simulation objective was evaluation of general LNAPL migration behavior and not the value of any specific parameter

Table of Scenarios for Evaluation of NAPL Migration in Vadose Zone and on Water Table

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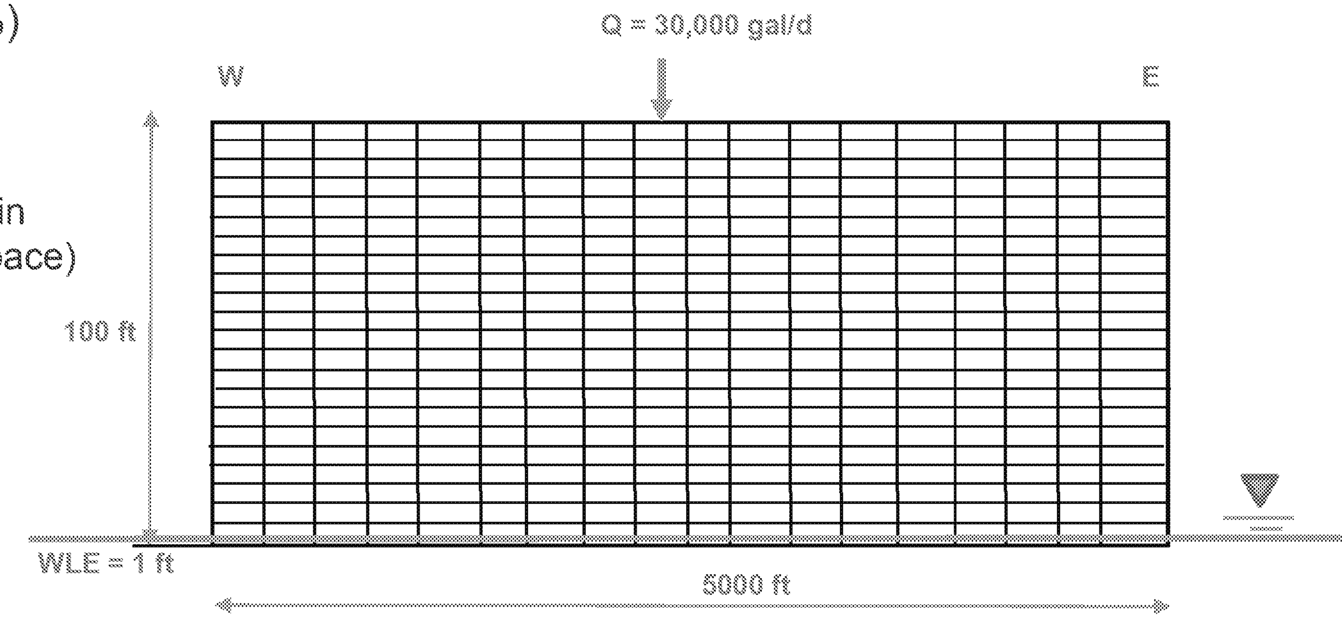
			Kh	Kz	A-N van G alpha	Porosity
Example	Source (ft^3/d)	Slope	(ft/d)	(ft/d)	(1/ft)	
Case 0	4,010 continuous	0%	*5,000*	*5,000*	1.5	0.1
Case 1	4,010 continuous	0%	5,000	***5***	1.5	0.1
Case 2	4,010 for ***200 days***	0%	5,000	5	1.5	0.1
Case 3	4,010 continuous	0%	***50***	5	1.5	0.1
Case3a	4,010 continuous	0%	50	5	***15***	0.1
Case 4	4,010 continuous	***3%***	5,000	5,000	1.5	0.1
Case 5	4,010 continuous	***3%***	5,000	***5***	1.5	0.1
Case 6	4,010 continuous	3%	5,000	5	1.5	***0.03***
Case 7	4,010 continuous	***10%***	5,000	5	1.5	0.03
Case 8	4,010 continuous	10%	5,000	***50***	1.5	0.03
Case 9	4,010 continuous	***3%***	5,000	5	1.5	***0.03 – 2-D***

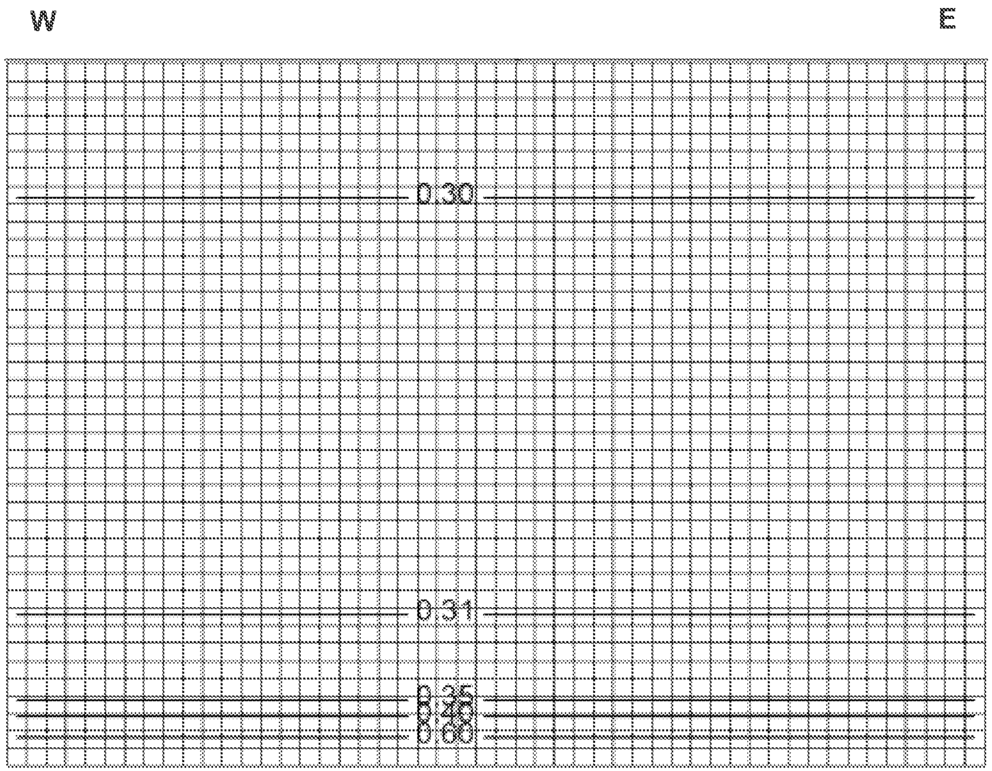
LNAPL (gasoline) Migration through a Horizontally Bedded Unsaturated Soil to a Horizontal Water Table

Setup

- Grid
  - Nx = Ny = 50; Nz = 40
  - Dx = Dy = 100 ft; Dz = 2.5 ft
- Hydraulic conductivity
  - Kx = 5,000 ft/d
  - Kz = 5,000 ft/d
- Porosity = 0.1 (10%)
- Saturation
  - S_{wr} = 0.3
  - S_{nr} = 0.14 (=0.2 in modified pore space)
- Continuous LNAPL source of 30,000 gallons/day (4,010 cu-ft/d)



Water Phase State (Saturations)

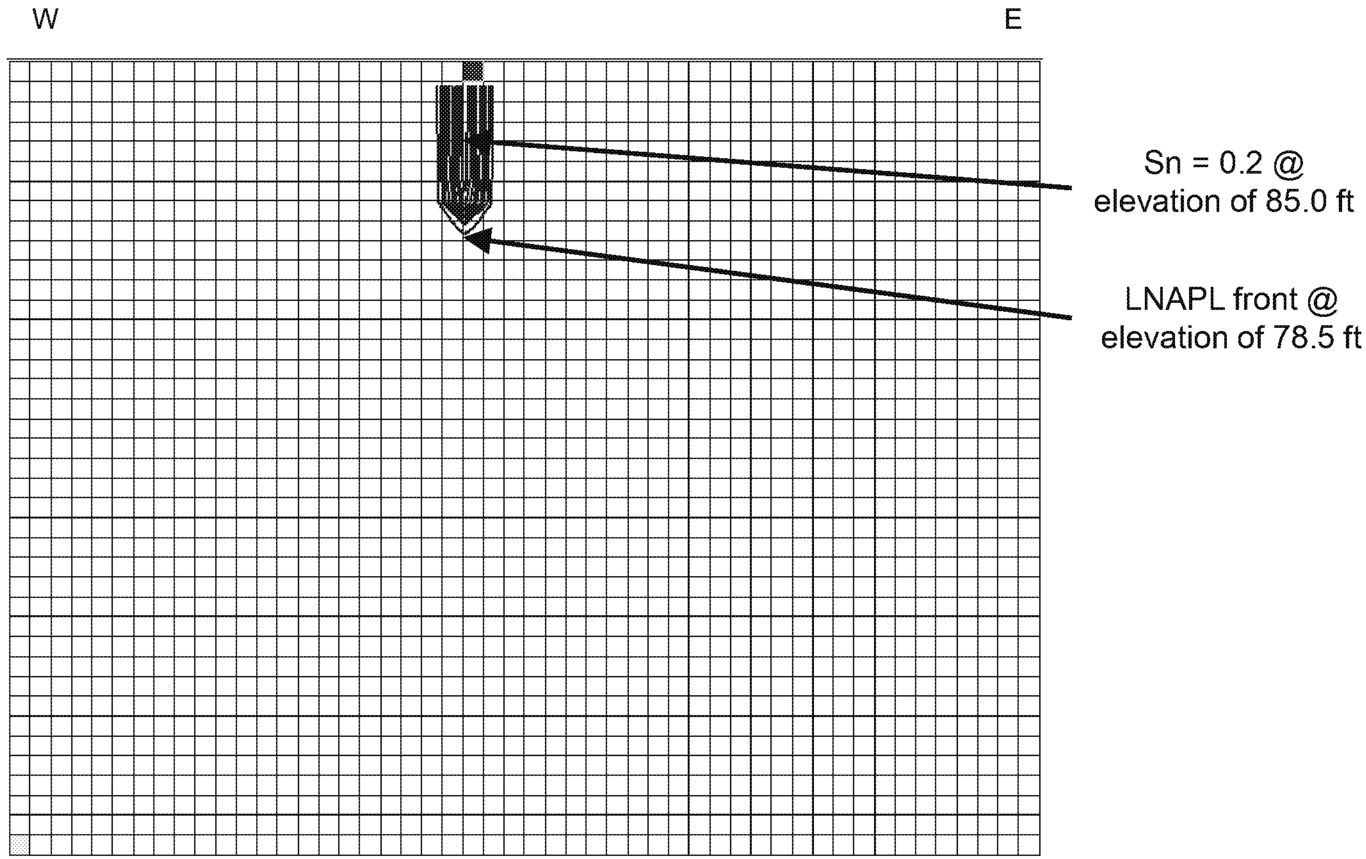


DX = 100 ft; DZ = 2.5 ft

Key point: (Result; Conclusion)

- Water saturation is at residual conditions within most of the domain; water phase saturations are not going to change with LNAPL flow
- Capillary rise simulated near the water table (S_w = 0.7 in bottom layer); reduces pore space for LNAPL intrusion, creating potential for more lateral migration at water table

LNAPL (gasoline) Saturations (T = 1 day)



DX = 100 ft; DZ = 2.5 ft

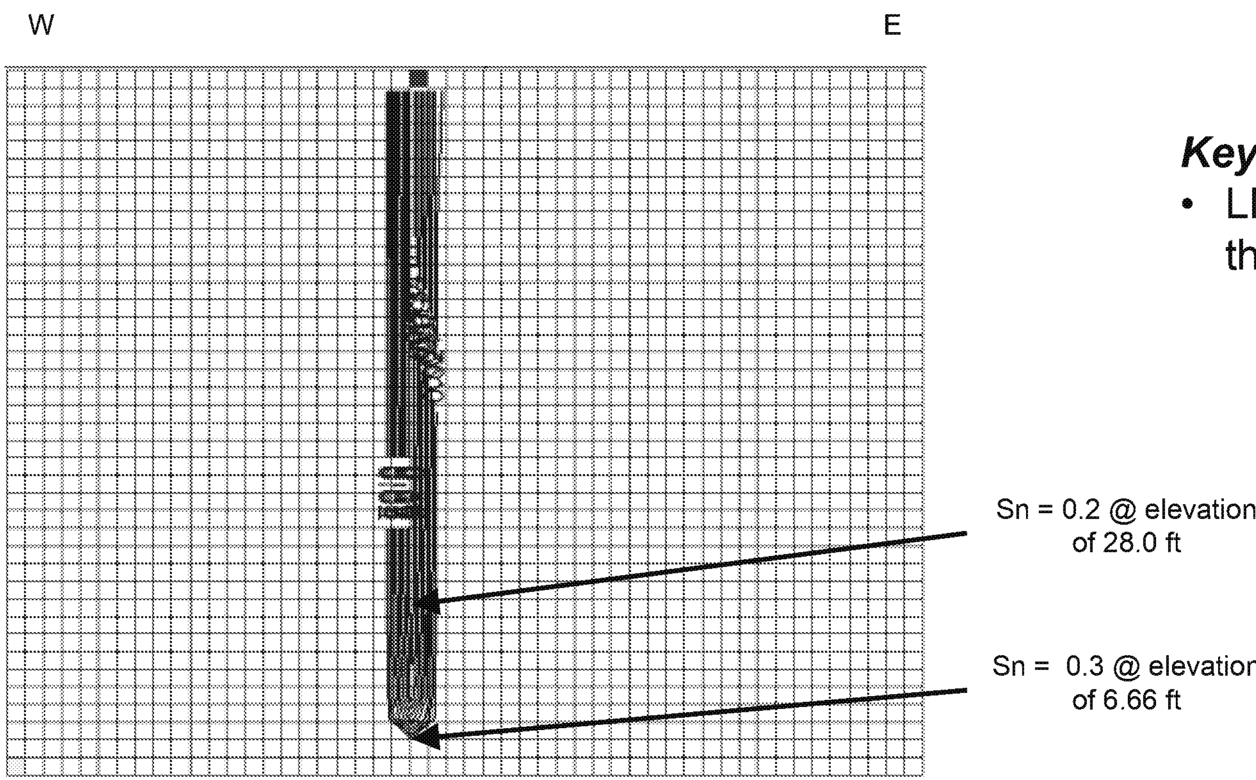
30,000 gallons
Kx / Kz = 1
Dip: Flat
Time = 1 Day

Key point:

- LNAPL has intruded about 22 feet vertically in 1 day

LNAPL (gasoline) Saturations (T = 5 days)

150,000 gallons
Kx / Kz = 1
Dip: Flat
Time = 5 Days

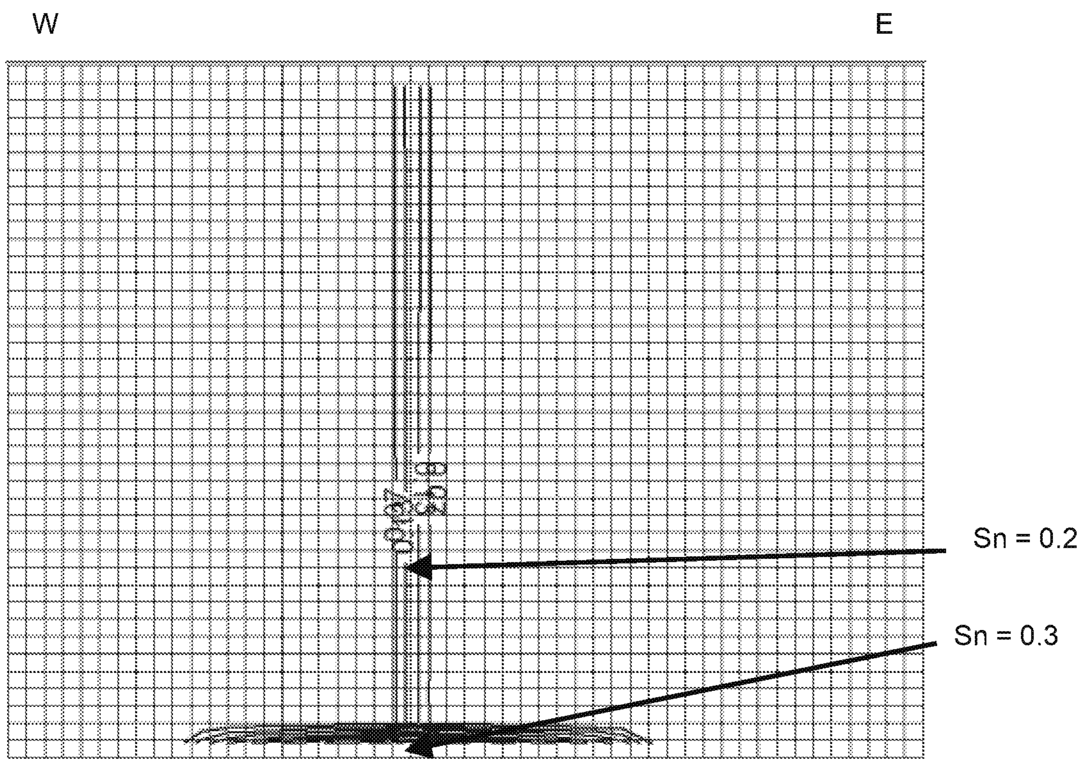


DX = 100 ft; DZ = 2.5 ft

Key point:
- LNAPL almost reaches the water table by 5 days

LNAPL (gasoline) Saturations (T = 6 days)

180,000 gallons
Kx / Kz = 1
Dip: Flat
Time = 6 Day



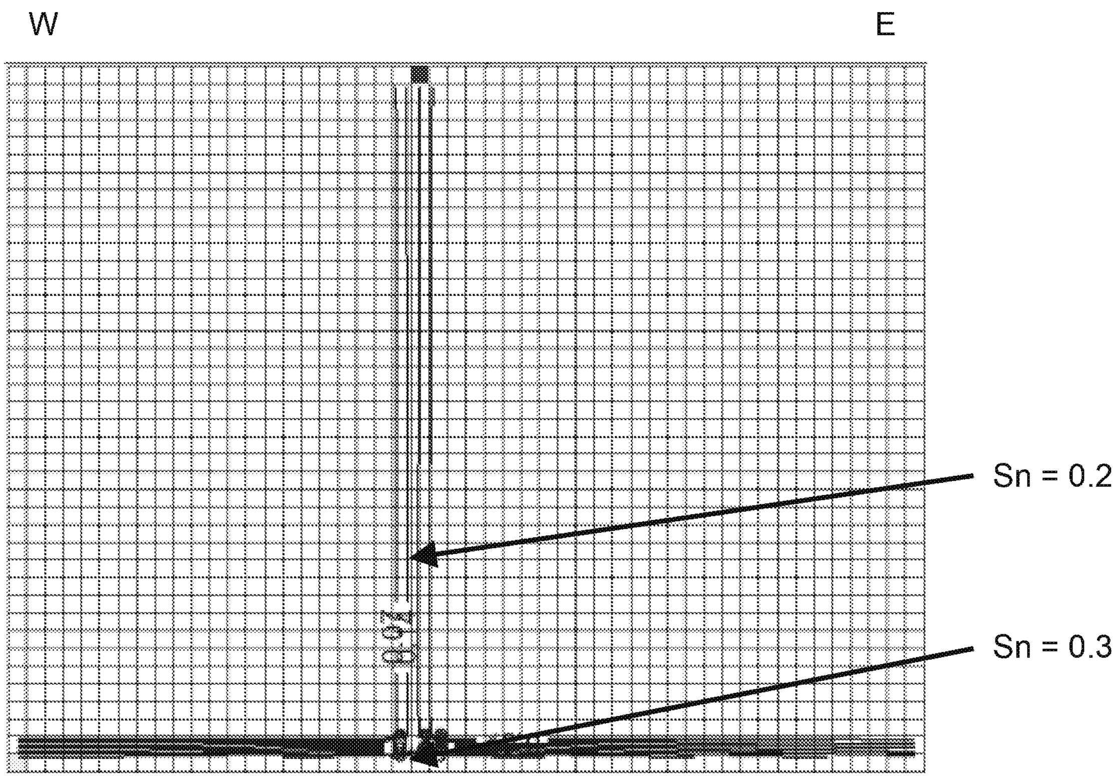
DX = 100 ft; DZ = 2.5 ft

Key point:

- LNAPL redistributes along the water table by 6 days
- LNAPL (saturation of 0.3) has spread radially by 1675 feet at the water table (in bottom layer of model)
- Sn never reaches full saturation
  - During vertical migration in unsaturated zone due to high K-values
  - During horizontal migration above capillary fringe due to higher saturation of water

LNAPL (gasoline) Saturations (T = 10 days)

300,000 gallons
Kx / Kz = 1
Dip: Flat
Time = 10 Days

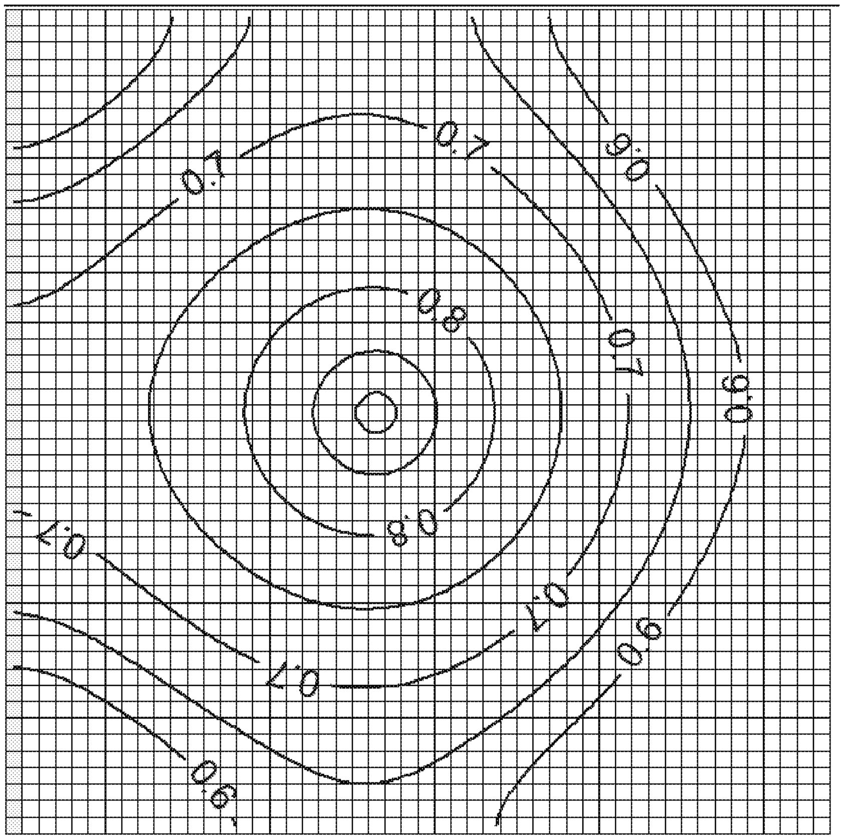


DX = 100 ft; DZ = 2.5 ft

Key point:

- LNAPL has reached boundary of domain by 10 days

LNAPL (gasoline) Saturations at Bottom of Domain (T = 10 days)



300,000 gallons
Kx / Kz = 1
Dip: Flat
Time = 10 Days

Note: Contours represent LNAPL saturation in modified porosity and should be scaled by 0.7 (= 1 – Sw) in bottom layer to represent Sn

Key point:

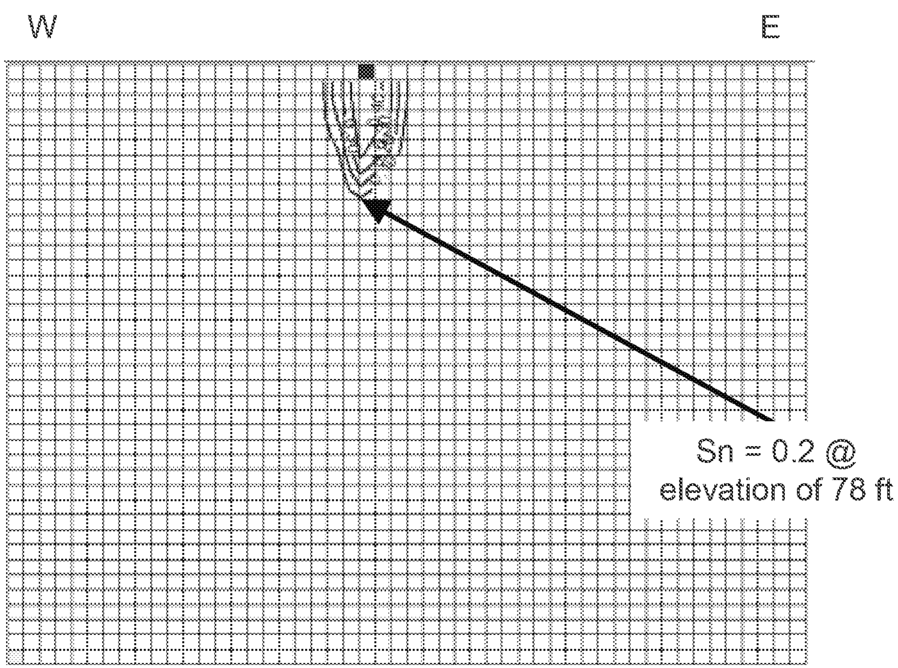
- LNAPL mounds on flat water table and migrates rapidly out of drain boundary to the west

Simulation Variations (Sensitivities)

1. Kz = 5 ft/d
2. Kz = 5 ft/d and source duration of 10 days releasing a total of 300,000 gallons followed by zero release for 200 days
3. Continuous release but with Kx = Ky = 50 ft/d; Kz = 5 ft/d
    a. Case 3a is the same as Case 3 with less capillarity: Van Genuchten alpha parameter changed from 1.5 to 15.0.

Case 1: (Kz = 5 ft/d): LNAPL (gasoline) Saturations (T = 10 day)

30,000 gal/day
300,000 gallons
Kx / Kz = 1,000
Dip: Flat
Time = 10 Days



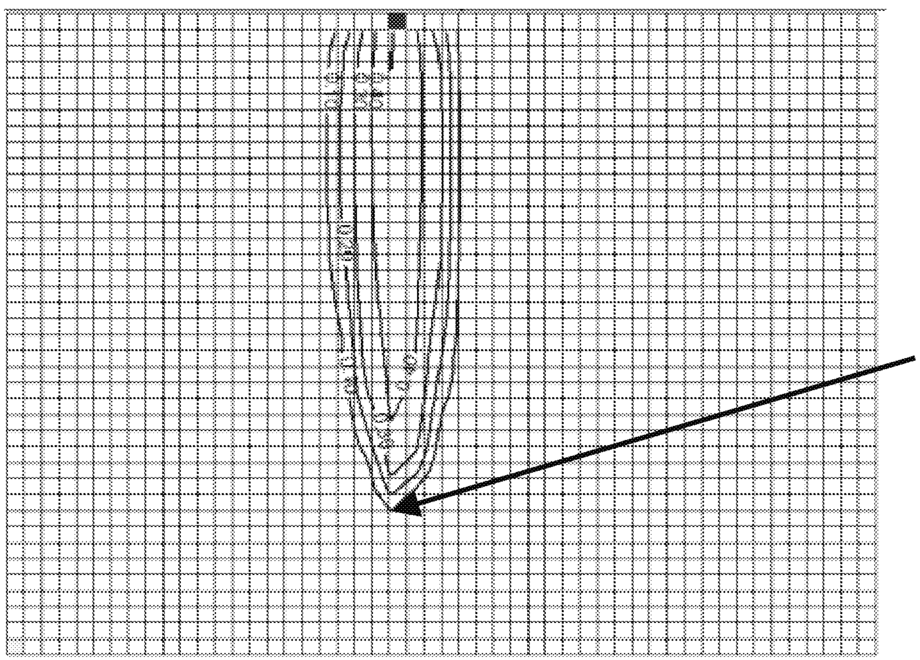
DX = 100 ft; DZ = 2.5 ft

Key points (Conclusions) :

- LNAPL travels 22 feet vertically in 10 days
- Kz = 5 ft/d compared to base case of Kz = 5,000 ft/d:
  - Slower vertical migration
  - More lateral (radial) migration
  - Higher LNAPL saturations
- Higher vertical anisotropy reduces vertical migration and enhances radial spreading in the vadose zone

Case 1: (Kz = 5 ft/d): LNAPL (gasoline) Saturations (T = 100 days)

W E



DX = 100 ft; DZ = 2.5 ft

Sn = 0.2 @ elevation of 24 ft

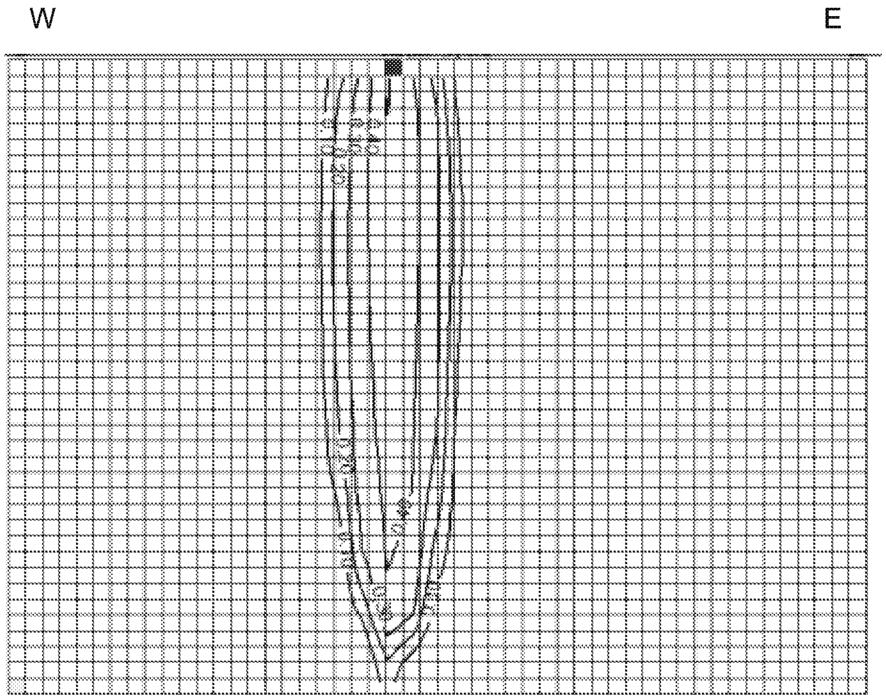
30,000 gal/day
3,000,000 gallons
Kx / Kz = 1,000
Dip: Flat
Time = 100 Days

Key point:

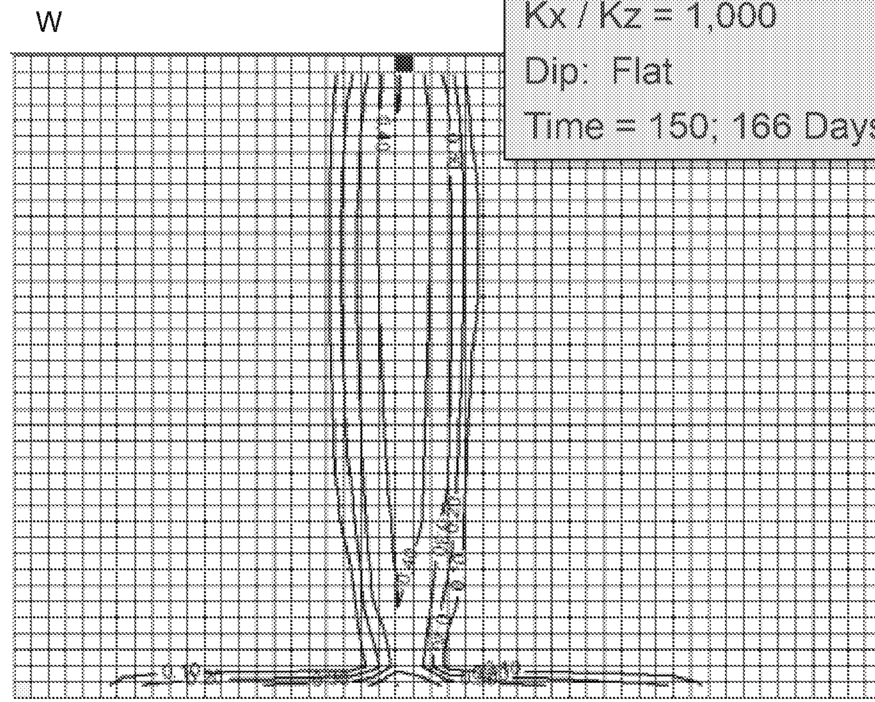
- LNAPL has moved vertically about 75 feet in 100 days (not yet reached water table)
- LNAPL has more radial spread than for Kz = 5,000 ft/d

Case 1: (Kz = 5 ft/d): LNAPL (gasoline) Saturations (T = 150 and 166 days)

3,000,000+ gallons
Kx / Kz = 1,000
Dip: Flat
Time = 150; 166 Days



150 days



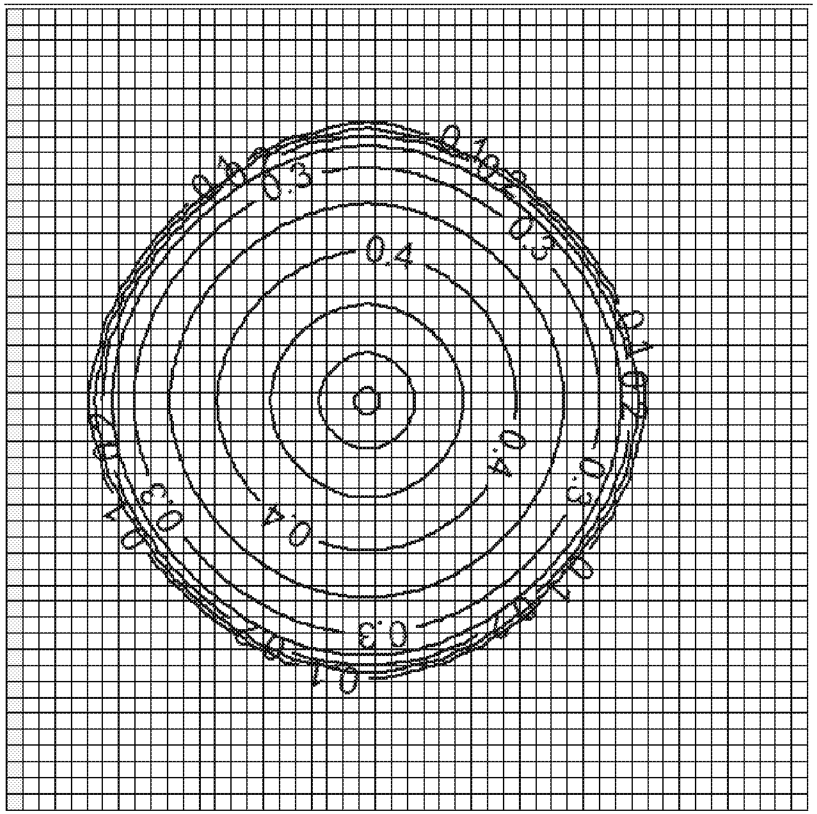
166 days

Key point:

- LNAPL takes 150 days to reach the water table but spreads rapidly once it reaches the water table.

Case 1: (Kz = 5 ft/d): LNAPL (gasoline) Saturations at Bottom of Domain (T = 166 days)

4,980,000 gallons
Kx / Kz = 1,000
Dip: Flat
Time = 166 Days



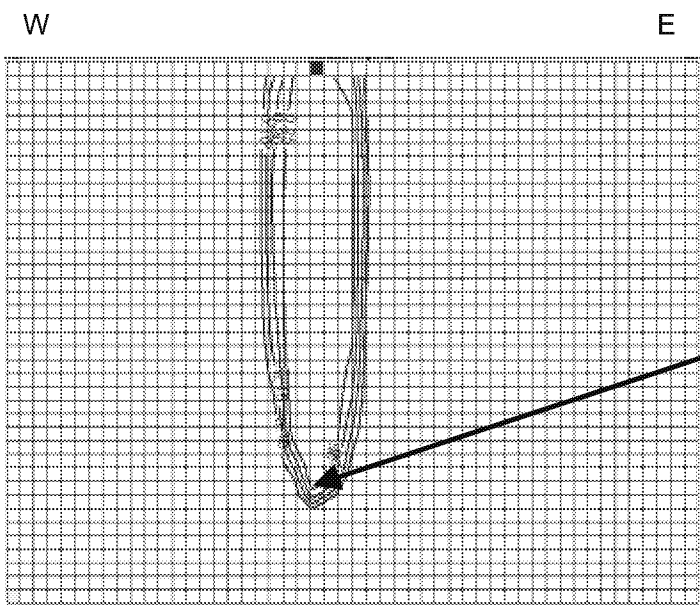
Contours represent LNAPL saturation in modified porosity and should be scaled by 0.7 (= 1 – Sw) in bottom layer to represent Sn

Key point:

- LNAPL mounds on flat water table
- 2-D areal simulation with no vertical flow will show LNAPL mounding very rapidly on base of model with flat bottom, which is unrealistically conservative

Case 2: (Kz = 5 ft/d and 100-day Source Duration): LNAPL (gasoline) Saturations (T = 166 days)

4,980,000 gallons
Kx / Kz = 1,000
Dip: Flat
Time = 166 Days



Sn = 0.2 @ elevation of 17.524 ft

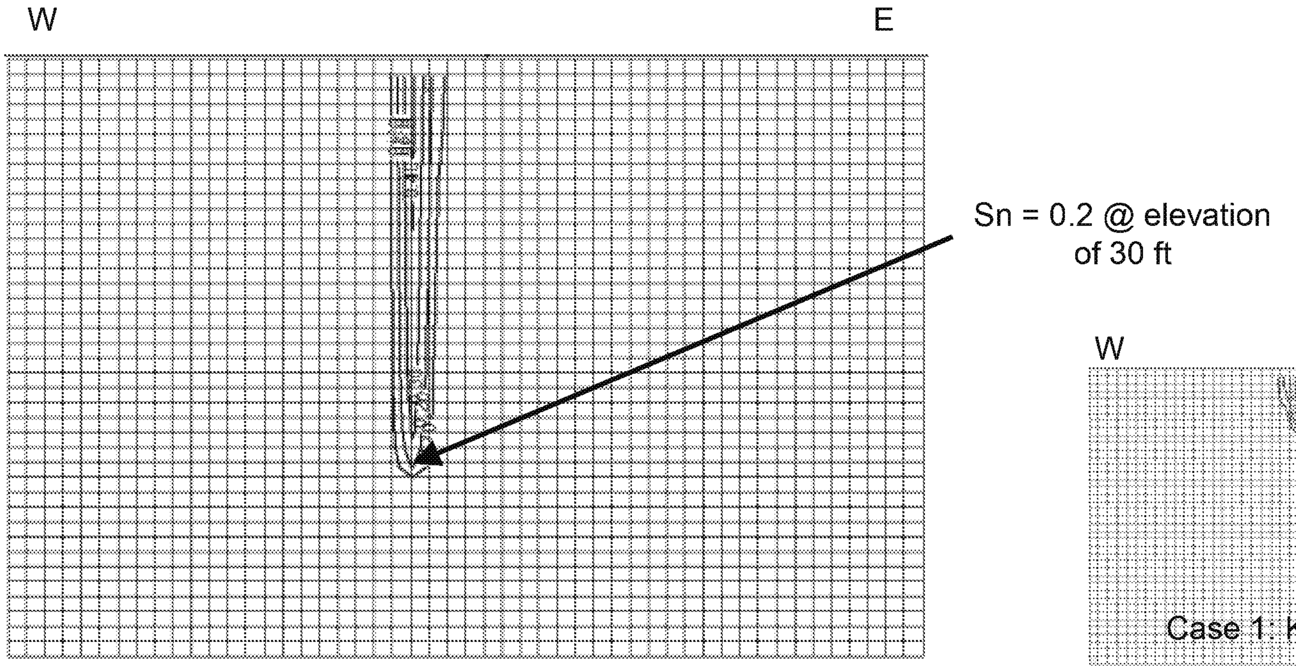
Note: At 100 days, this simulation has the same result as for previous case at 100 days.

Key point (Conclusion):

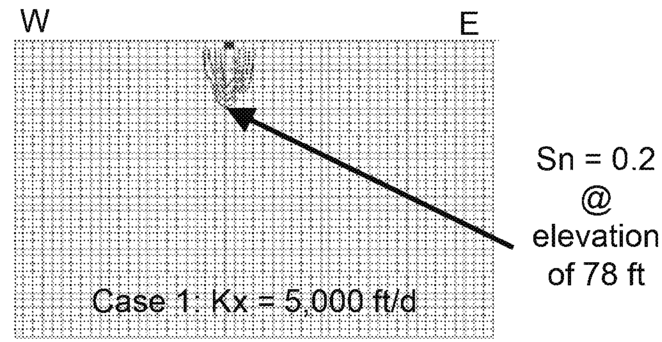
- LNAPL approaches residual saturation and does not reach the water table when source is shut off at 100 days, with only slight redistribution and drainage from the 100-day contours
- LNAPL movement in the vadose zone reduces significantly once the source is turned off

Case 3: (K_x = 50 ft/d; K_z = 5 ft/d):
LNAPL (gasoline) Saturations (T = 10 days)

300,000 gallons
Kx / Kz = 10
Dip: Flat
Time = 10 Days



DX = 100 ft; DZ = 2.5 ft



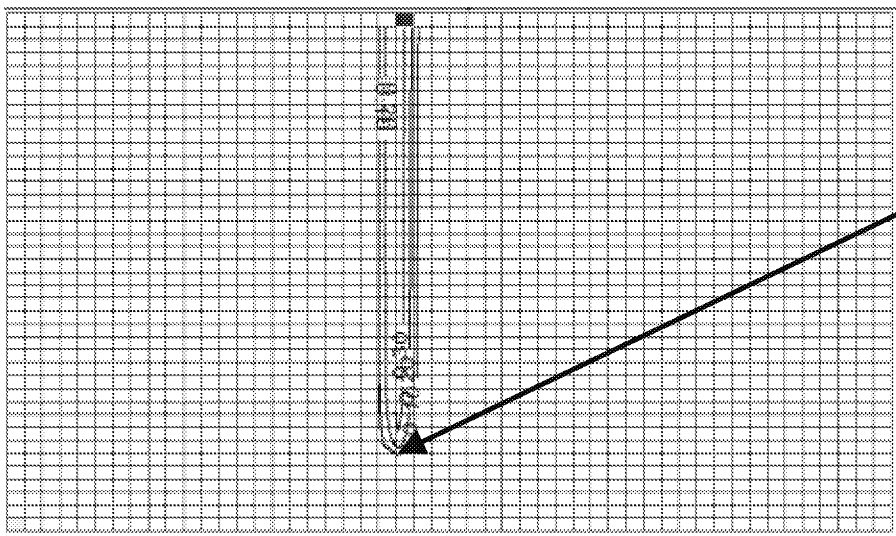
Key point (Conclusion):

- LNAPL horizontal spread is less and vertical travel is more than for Case 1 (with K_x = 5,000 ft/d and K_z = 5 ft/d shown in inset)
- Higher vertical anisotropy reduces vertical migration and enhances radial spreading in the vadose zone (decreasing K_h increases vertical flow)

Case 3a: (Case 3 with less capillarity): LNAPL (gasoline) Saturations (T = 10 days)

300,000 gallons
Kx / Kz = 10
Dip: Flat
Time = 10 Days

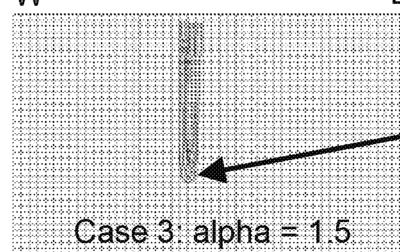
W
Case 3a: alpha = 15.0
E



DX = 100 ft; DZ = 2.5 ft

Sn = 0.2 @ elevation of 15 ft

W
E



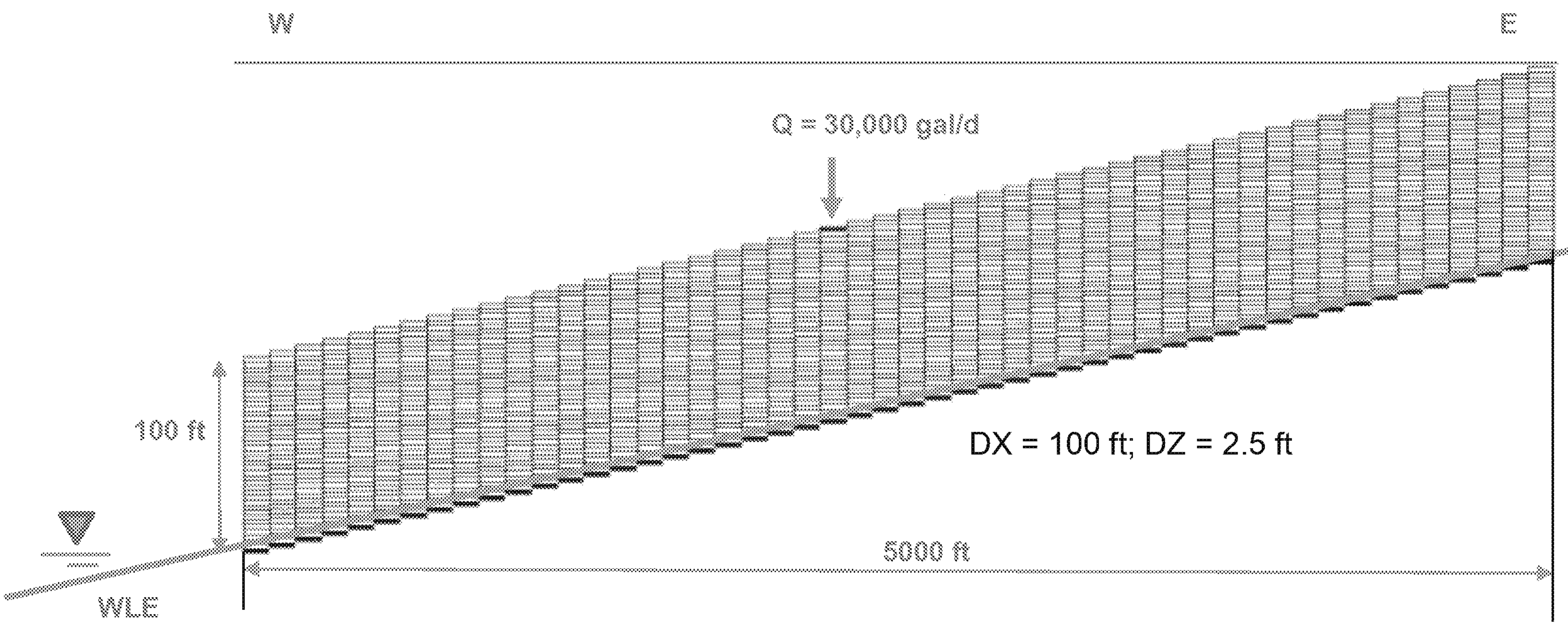
Sn = 0.2 @ elevation of 30 ft

***Key point** (Conclusion):*

- LNAPL vertical travel is slightly more with less capillarity than for Case 3 that has higher capillarity
- Slight sensitivity to capillarity of LNAPL (migrated additional 15 feet in 10 days for lower capillarity)

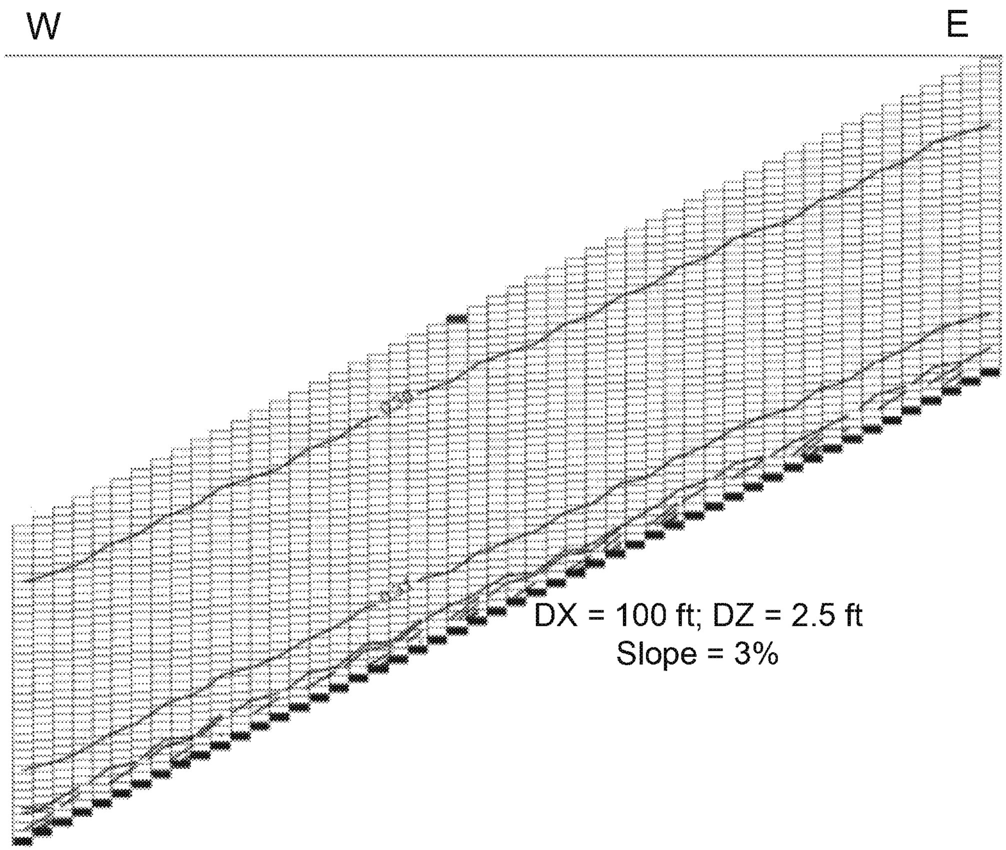
Case 4: LNAPL (gasoline) Migration through a Sloping Bedded Unsaturated Soil or along a Sloping Water Table

- Setup
  - Kx = Kz = 5,000 ft/d
- Slope = 3%.
- WLE = 1 ft along west, rising with slope of 3% toward the east
- Continuous LNAPL source



Note: LNAPL source was kept in middle of domain for consistency with previous simulations

Case 4: Sloping Bed at 3% (1.7 degrees): Water Phase State (Saturations)

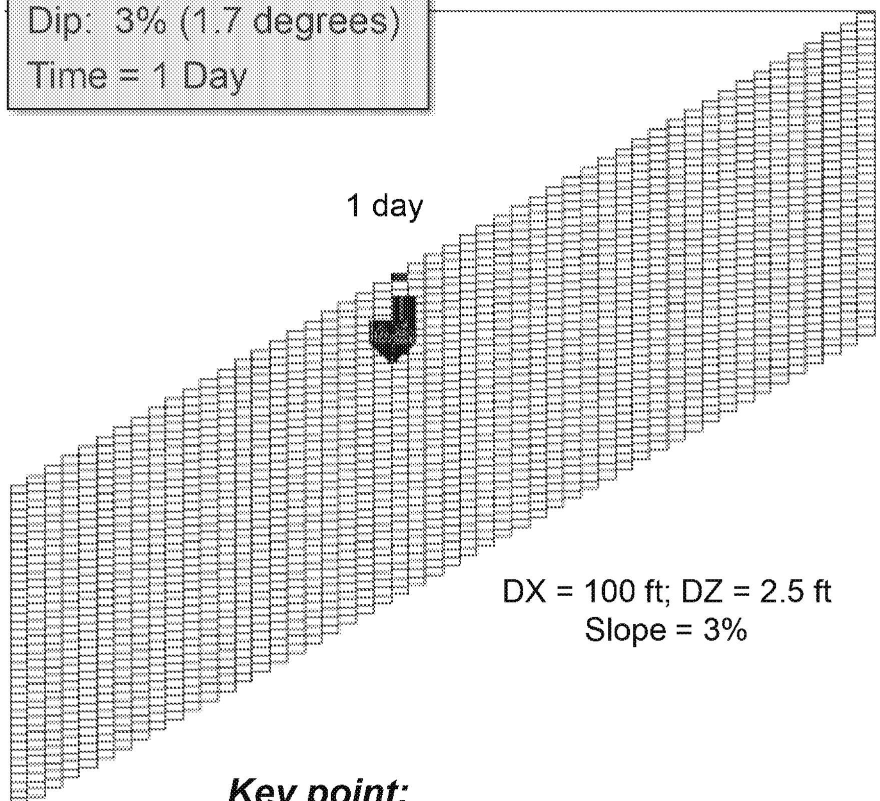


Key point:

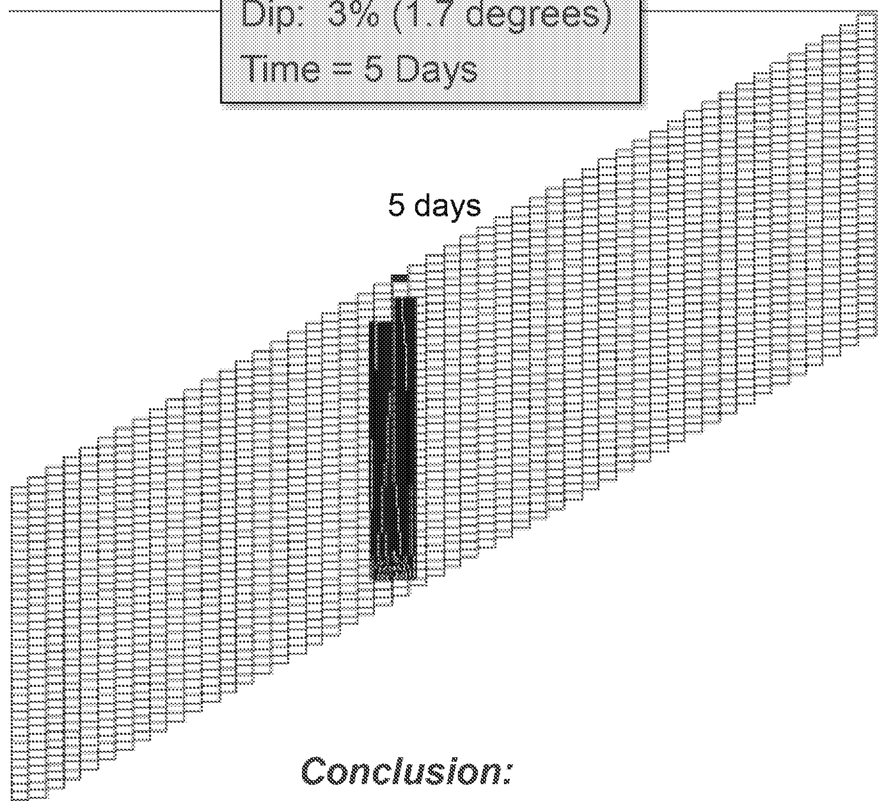
- Water saturation is at residual conditions along most of the domain with some capillary rise above the water table

Case 4: Sloping Bed at 3%: LNAPL (gasoline) Saturations (T = 1 and 5 days)

30,000 gallons
Kx / Kz = 1
Dip: 3% (1.7 degrees)
Time = 1 Day



150,000 gallons
Kx / Kz = 1
Dip: 3% (1.7 degrees)
Time = 5 Days



Key point:

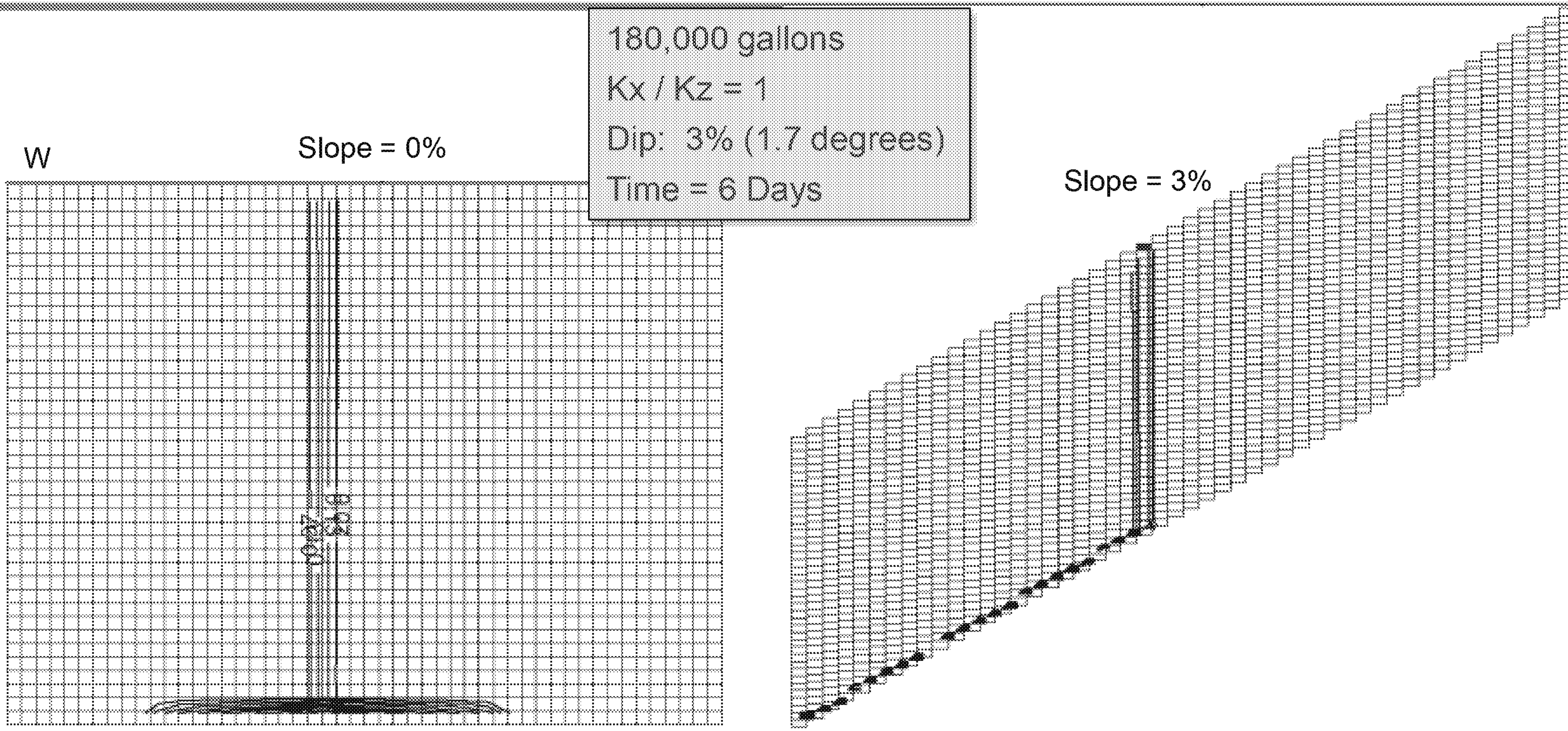
- LNAPL has intruded about the same amount at 1 and 5 days as for a horizontal grid

Conclusion:

- Bedding slope does not influence LNAPL movement when Kz is very high

Case 4: Sloping Bed at 3%: LNAPL (gasoline) Saturations (T = 6 days)

180,000 gallons
Kx / Kz = 1
Dip: 3% (1.7 degrees)
Time = 6 Days



Key point (Conclusion):

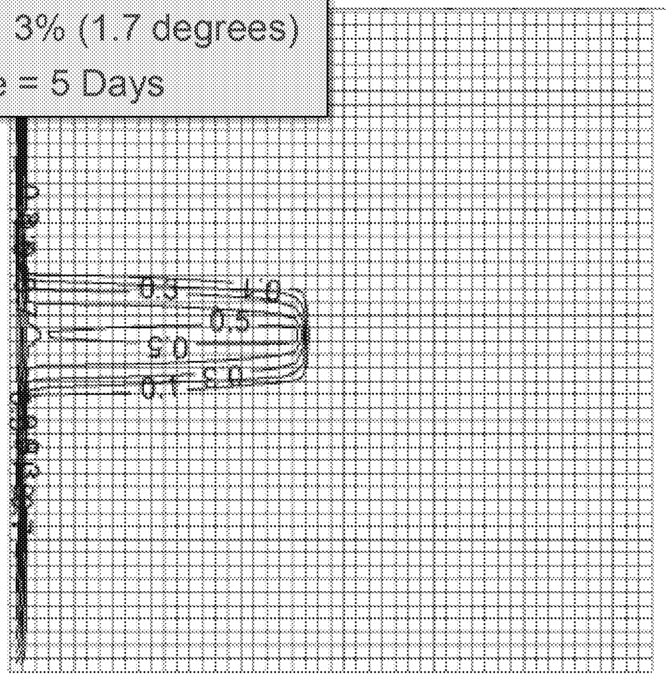
- LNAPL reached boundary on sloping water table by 6 days (had spread radially 1,675 feet on flat water table)
- LNAPL migration along a sloping water table is faster than on a flat water table

Case 4: Sloping Bed at 3%: LNAPL (gasoline) Saturations at Bottom of Domain

NAVFAC

150,000 gallons
Kx / Kz = 1
Dip: 3% (1.7 degrees)
Time = 5 Days

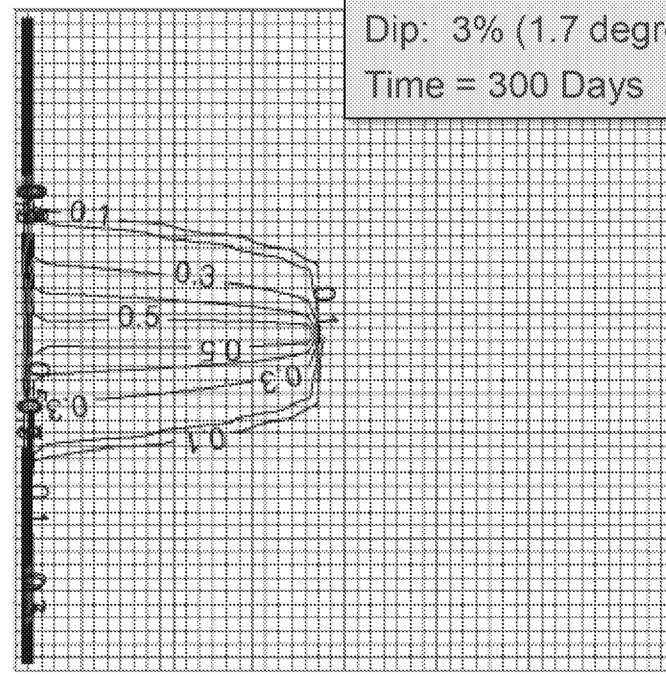
5 days



Contours represent LNAPL saturation in modified porosity and should be scaled by 0.7 (= 1 – Sw) in bottom layer to represent Sn

300 days

9,000,000 gallons
Kx / Kz = 1
Dip: 3% (1.7 degrees)
Time = 300 Days



Key Points (Conclusion):

- LNAPL migrates with considerable lateral spreading along the sloping water table due to superposition of ambient flow and mounding
- 2-D areal simulation with no vertical flow will show similar LNAPL movement at base of sloping bottom and is unrealistically conservative

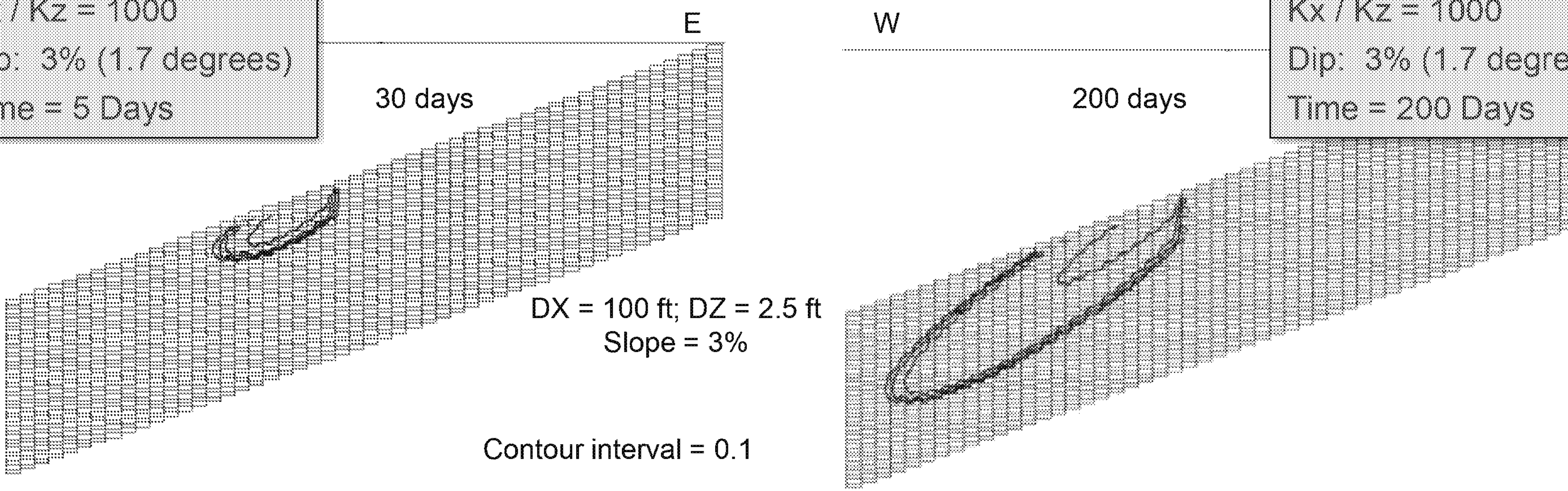
Simulation Variations (Sensitivities)

5. Kz = 5 ft/d
6. Kz = 5 ft/d and porosity = 0.03
7. Kz = 5 ft/d; porosity = 0.03; 10% slope
8. Kz = 50 ft/d; porosity = 0.03; 10% slope
9. Two-dimensional representation of simulation 6 above

Case 5: (Slope = 3%; Kz = 5 ft/d):
LNAPL (gasoline) Saturation

900,000 gallons
Kx / Kz = 1000
Dip: 3% (1.7 degrees)
Time = 5 Days

6,000,000 gallons
Kx / Kz = 1000
Dip: 3% (1.7 degrees)
Time = 200 Days

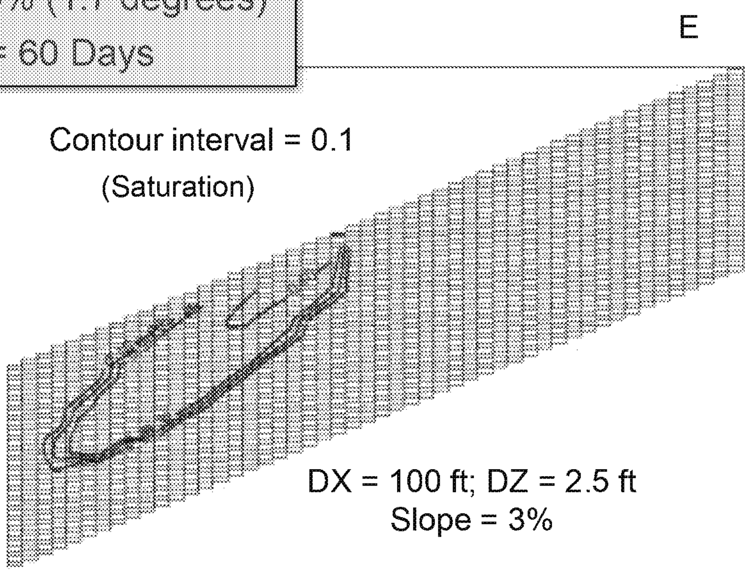


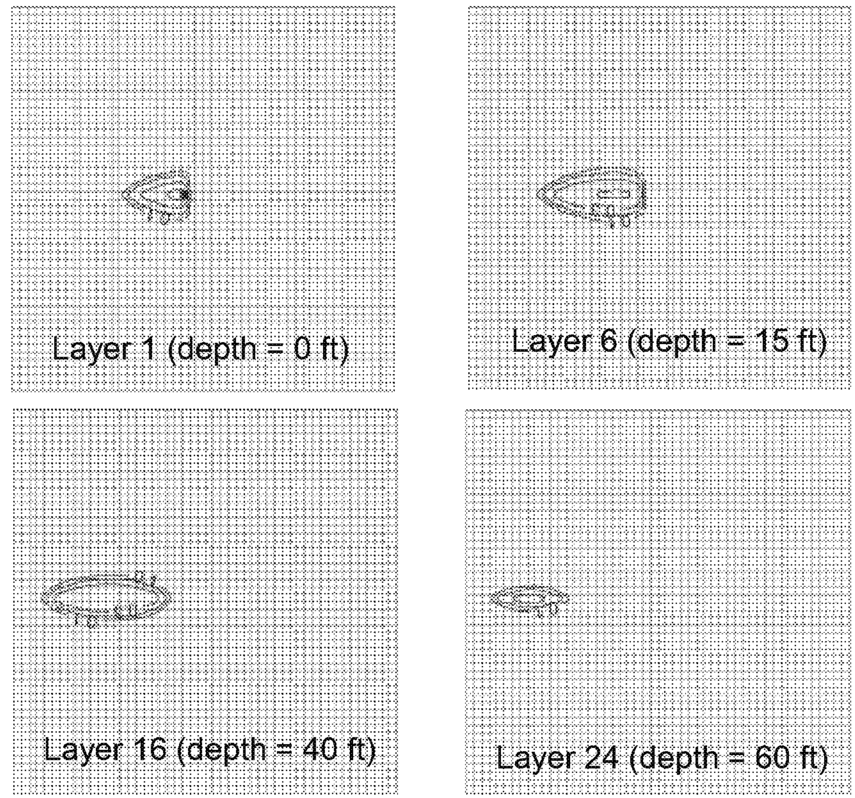
Key points (Conclusions):

- Movement is slower with higher saturation buildup and more lateral migration than for Kz = 5,000 ft/d case
- A total of 6 million gallons of LNAPL have entered soil in 200 days and not reached lateral boundary or water table
- Sloping bed causes lateral migration in the direction of slope when there is high material anisotropy
- Migration is downward and laterally

Case 6: (Slope = 3%; Kz = 5 ft/d; Porosity = 0.03): LNAPL (gasoline) Saturation at 60 days

1,800,000 gallons
Kx / Kz = 1000
Dip: 3% (1.7 degrees)
Time = 60 Days



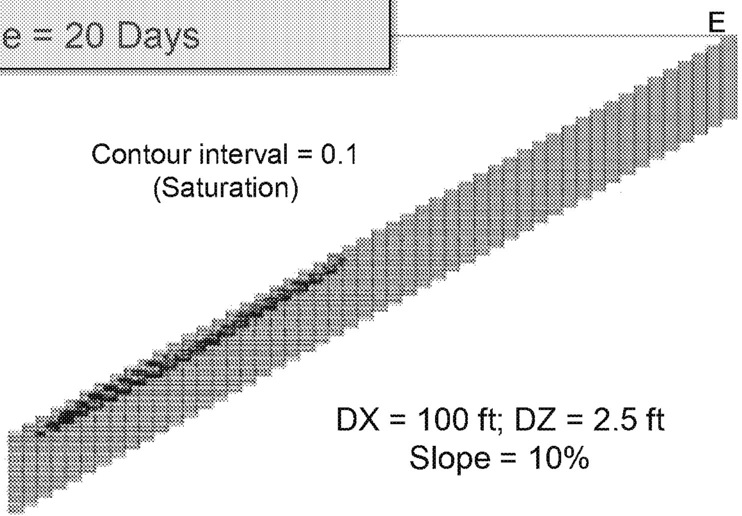


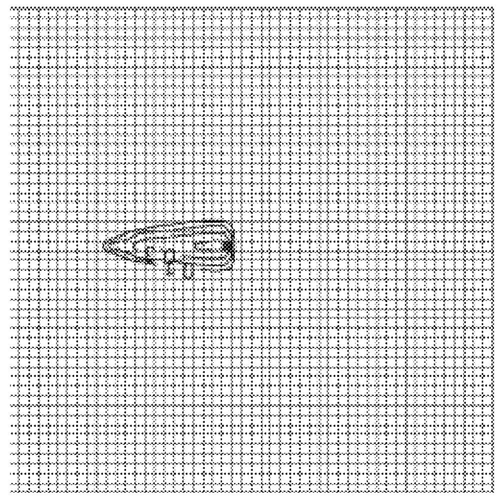
Key point (Conclusion):

- LNAPL plume at 60 days with porosity of 0.03 is similar to plume at 200 days with porosity of 0.1
- LNAPL movement scales linearly with porosity

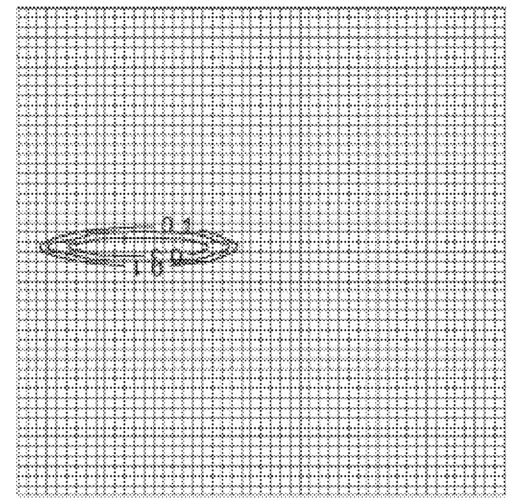
Case 7: (Slope = 10%; Kz = 5 ft/d; Porosity = 0.03): LNAPL (gasoline) Saturation at 20 days

600,000 gallons
Kx / Kz = 1000
Dip: 10% (5.7 degrees)
Time = 20 Days





Layer 1 (depth = 0 ft)



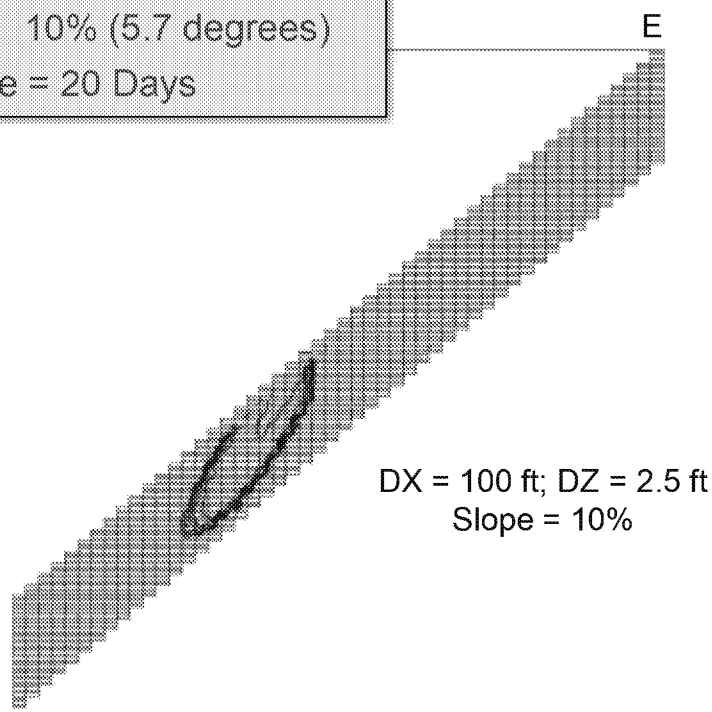
Layer 6 (depth = 15 ft)

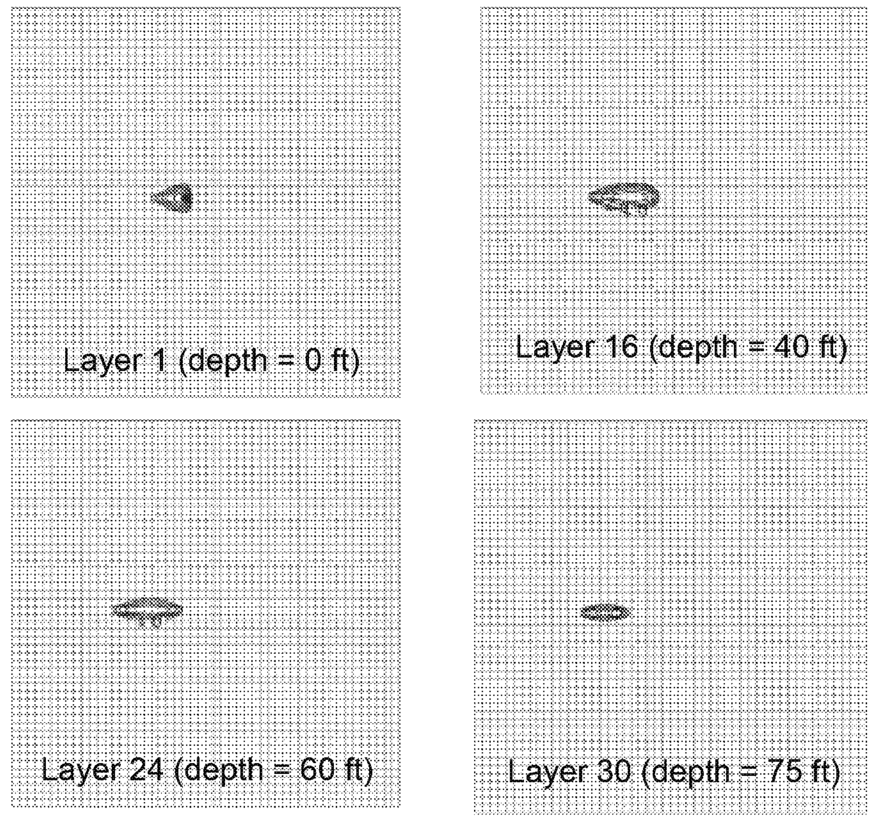
Key points (Conclusions):

- Plume migration is more aligned with the bedding slope than for a 3% slope
- Lateral movement of plume in 20 days with a 10% slope is similar to lateral movement in 60 days with a 3% slope
- For steeper bedding slope, the plume migration is quicker and more aligned with bedding slope

Case 8: (Slope = 10%; Kz = 50 ft/d; Porosity = 0.03): LNAPL (gasoline) Saturation at 20 days

600,000 gallons
Kx / Kz = 1000
Dip: 10% (5.7 degrees)
Time = 20 Days





Key point (Conclusion):
- Less anisotropy allows for deeper migration
- There is interaction between dip angle and anisotropy – timing may also be significant

Case 9: (2-D; Slope = 3%; Kz = 5 ft/d; Porosity = 0.03): LNAPL (gasoline) Saturation at 15 days

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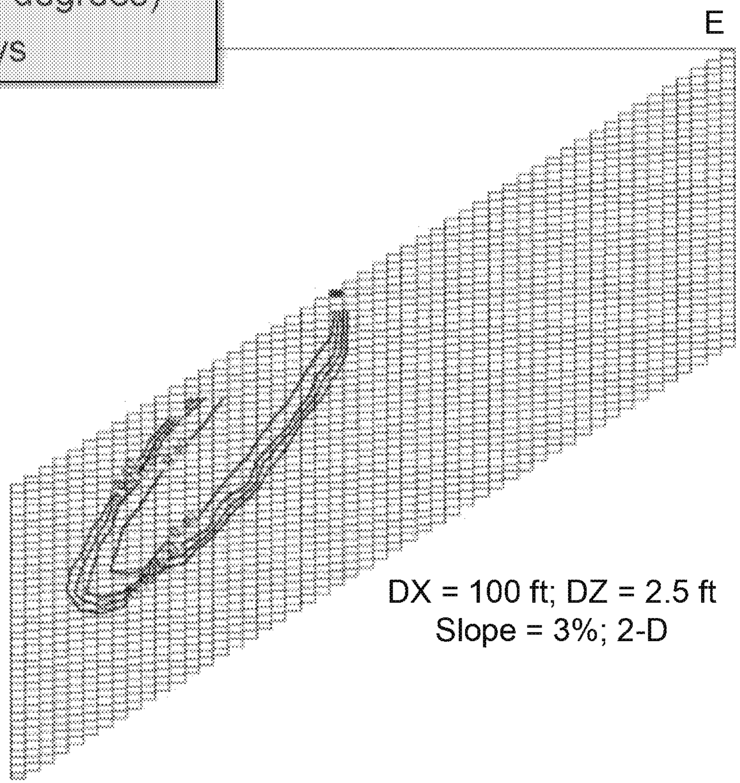
450,000 gallons
Kx / Kz = 1000
Dip: 10% (5.7 degrees)
Time = 15 Days



***Key point* (Conclusion):**

- Simulated lateral migration is as much (or larger for the Sn = 0.4 contour) within 15 days than for a fully 3-D analysis within 60 days
- 2D is unreasonably conservative – 4 times more conservative than a 3-D analysis for this case
- 2-D assumptions are violated for Red Hill tank conditions… 2-D is appropriate for line sources/sinks and not point sources/sinks

Observations - LNAPL Simulations

- Water phase is at residual saturation through most of the soil column
- Higher vertical anisotropy reduces vertical migration and enhances radial spreading or flow along sloped bedding plane in the vadose zone
- Bedding slope impact
  - No impact when Kz is high
  - LNAPL migration impacted by bedding slope and anisotropy combination
- LNAPL migration reduces significantly once source is turned off
- LNAPL migration in the vadose zone is only slightly sensitive to capillarity
- 2-D areal or vertical analyses are unreasonably conservative

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Key Parameters for LNAPL Migration Evaluations

Key Parameters for LNAPL Migration in Vadose Zone

NAVFAC

- ***Porosity:*** Migration distance scales inversely with porosity
- ***Residual or capillary water saturation:*** Same effect as reducing porosity
- ***Vertical anisotropy and Bed Slope:*** Combination determines migration behavior. Higher vertical anisotropy reduces vertical migration for flat bedding plane
- ***Vertical hydraulic conductivity:*** Quicker vertical movement with higher vertical conductivity
- **2-phase Air – NAPL (AN) constitutive relationships:**
  - Higher capillarity causes less vertical migration
  - Higher relative permeability exponent causes less migration
  - Generally not very sensitive
- ***Residual LNAPL saturation:*** Sensitive for drainage after release has stopped. During imbibition, saturations are higher than residual so they are not of consequence.

Key Parameters for LNAPL Migration on Water Table

- ***Water table slope:*** Migration is the combined result of ambient gradients and mounding at the source
- ***Horizontal hydraulic conductivity:*** Quicker horizontal movement with higher horizontal hydraulic conductivity

Naval Facilities Engineering Command
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Demonstration of Simulation Approach at Red Hill to Parameter Evaluation and Application to Hypothetical Sudden Catastrophic Release Using a Test Model

Evaluate 2014 Spill at Facility Using Test Model

The simulations are a test case to demonstrate the proposed simplified approach for Red Hill LNAPL evaluation.

- ***This is for demonstration purposes only, and future efforts will be aligned with the Navy's LNAPL modeling objectives***

- Vertical extent/depth of 2014 release in the vadose zone (it did not reach groundwater)
- Water Table Slope = flat
- 2014 Release Volume = 27,000 gallons (jet fuel)
- 2014 Release Duration = 30 days
- Release rate = 27,000/30 = 900 gallons/day = 120.3 cu-ft/day (30.075 cu-ft/d over 4 cells)
- Distance from tanks to S. Halawa Valley saprolite = 900 ft
- Distance from tanks to Moanalua Valley saprolite = 1500 ft
- Distance from lower tanks to Red Hill Shaft (end) = 1500 ft
- Release area = 100 feet x 100 feet
- Grid horizontally refined from before to be 50 ft x 50 ft size (same Nx and Ny)
- Source was moved to west; distance between source and east boundary = 300 feet

Some Parameters for LNAPL and Water

- Density of water = 1
- Density of jet fuel = 0.8
- Viscosity of water = 0.89 cP
- Viscosity of jet fuel = 1.19 cP

$$K_n = \frac{\rho_n}{\mu_n}\frac{\mu_w}{\rho_w}K_w = 0.6K_w$$

- Porosity = 0.03
- Water residual saturation = 0.3
- LNAPL residual saturation = 0.14

Some More Parameters for LNAPL and Water

- Interfacial tension for air water = 69.9 dynes/cm = 0.0699 N/m
- Interfacial tension for air LNAPL = 25 dynes/cm = 0.025 N/m
- Interfacial tension for LNAPL water = 15.7 dynes/cm = 0.0157 N/m

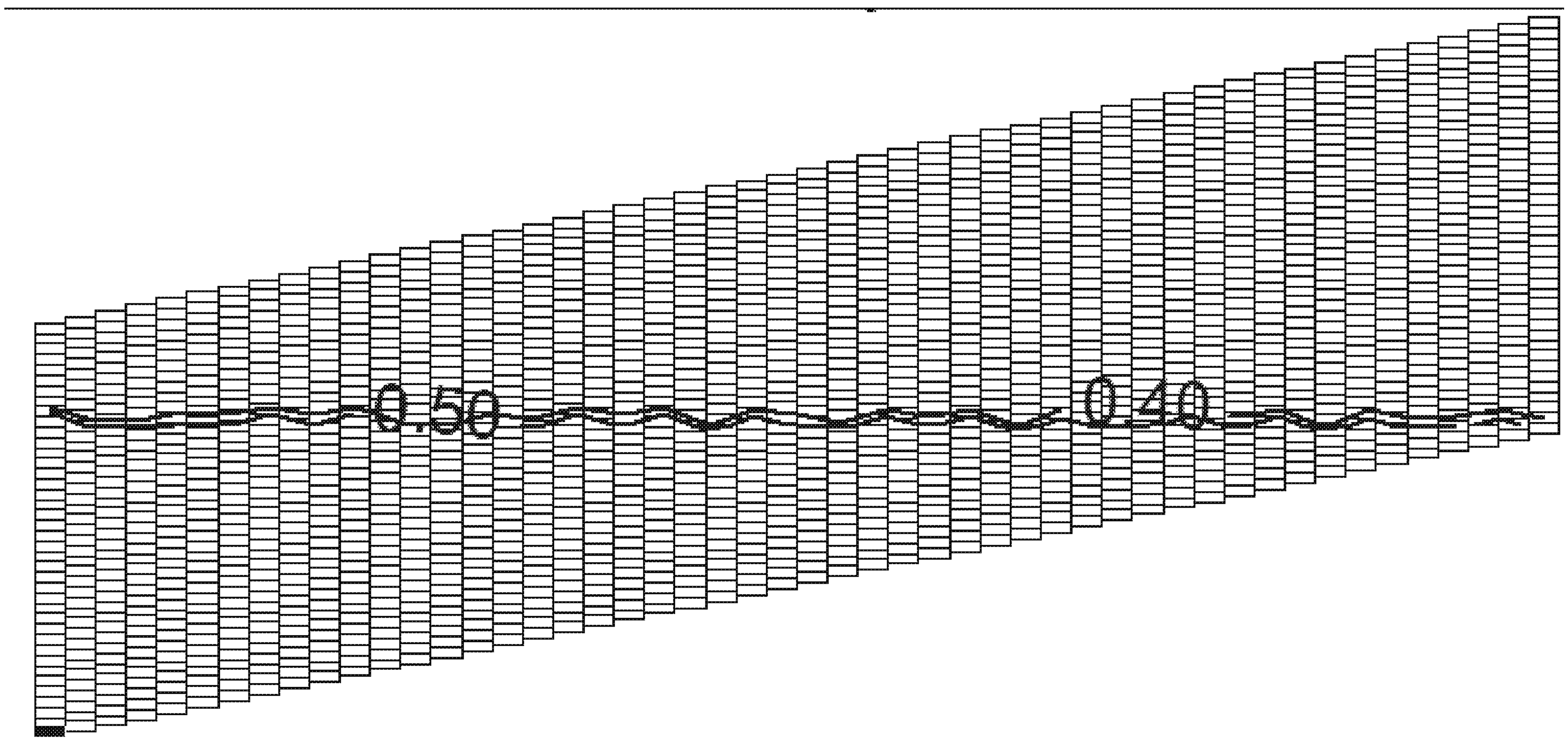
$$\beta_{nw} = \frac{\sigma_{aw}}{\sigma_{nw}} = 4.45 \qquad \beta_{an} = \frac{\sigma_{aw}}{\sigma_{an}} = 2.8$$

- van Genuchten Alpha for air-water system = 0.44 (1/ft)
- van Genuchten Beta = 2.68
- Brooks Corey "n" = 4.19 (generally related to van Genuchten parameters as):

$$n = 1 + \frac{2\beta}{(\beta - 1)}$$

- Scaled Alpha for LNAPL-water system = 0.44*4.45 = 1.96 (1/ft)
- Scaled Alpha for air-LNAPL system = 0.44*2.8 = 1.23 (1/ft)

Bedding Slope of 3% with Flat Water Table: Water Saturation Results

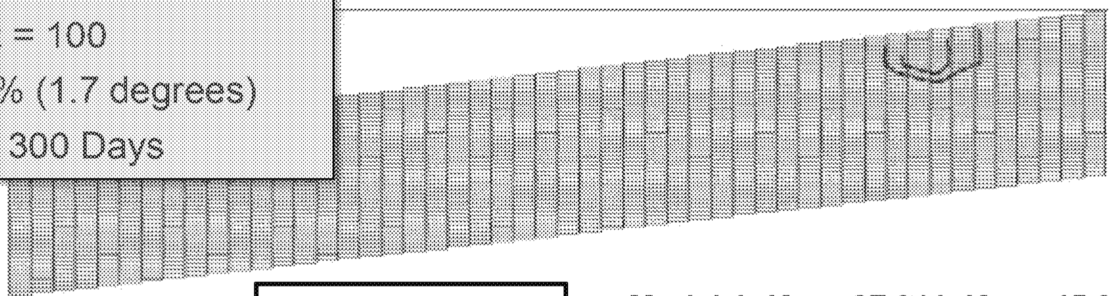


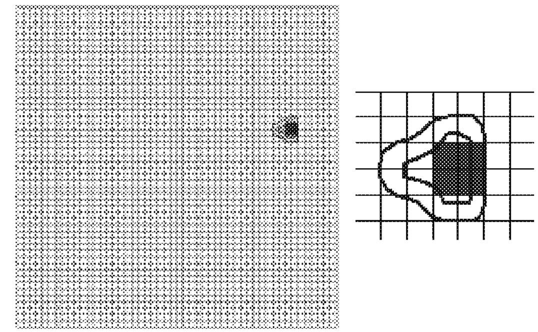
Calibration to 2014 Spill Information

- No indication that the 2014 release spread under adjacent tanks based on soil gas data – **radial spreading less than 100 ft from edge of tank**
- Thermal profile of RHMW02 indicates vertical extent well above water table – **vertical migration less than to water table**
- For K_{wx} = 4,500 ft/d; K_{nx} = 2,700 ft/d
  K_{wy} = 1,500 ft/d; K_{ny} = 900 ft/d
  K_{wz} = 8.5 ft/d; K_{nz} = 5 ft/d – *does not calibrate test model*
- K_{nz} = 27 ft/d calibrates low end (model 1)
- K_{nz} = 270 ft/d calibrates high end (model 2)

2014 Spill Calibrated LNAPL Plume

27,000 gallons
Kx / Kz = 100
Dip: 3% (1.7 degrees)
Time = 300 Days



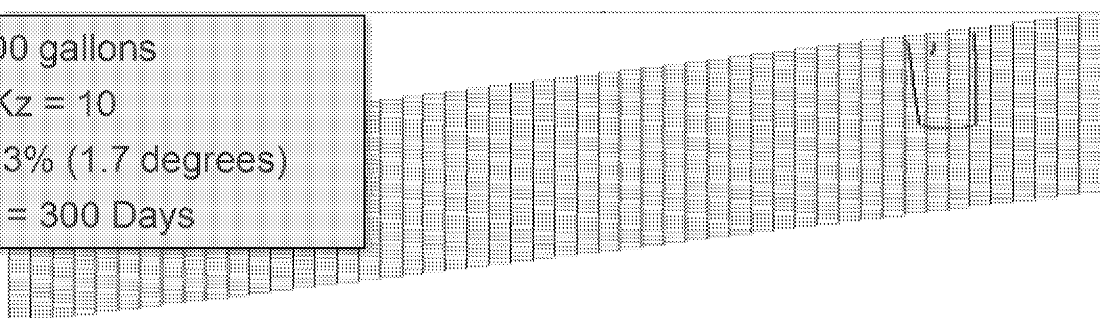


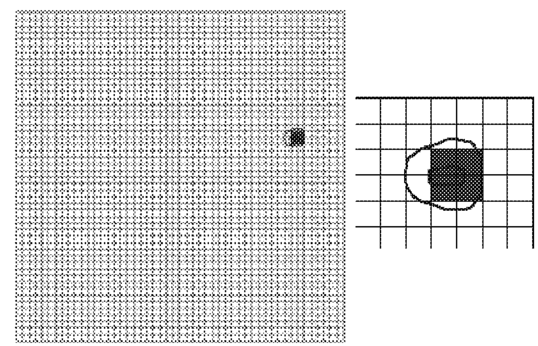
Test Model 1

Model 1: K_{nz} = 27 ft/d; K_{wz} = 45 ft/d

- **Vertical travel distance = 30 ft**
- **Horizontal travel distance = 100 ft longitudinal and 50 feet lateral**

27,000 gallons
Kx / Kz = 10
Dip: 3% (1.7 degrees)
Time = 300 Days





Test Model 2

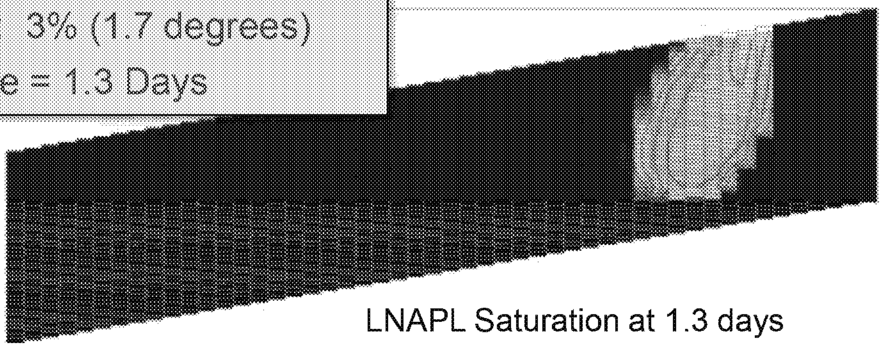
Model 2: K_{nz} = 270 ft/d; K_{wz} = 450 ft/d

- **Vertical travel distance = 55 ft**
- **Horizontal travel distance = <50 ft longitudinal and 50 feet lateral**

What catastrophic continuous release of LNAPL reaches the water table and when?

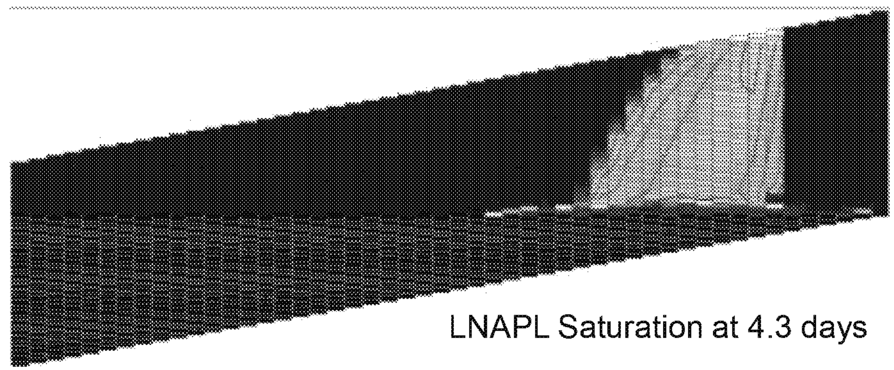
351,000 gallons
Kx / Kz = 100
Dip: 3% (1.7 degrees)
Time = 1.3 Days

Test Model 1: K_{wz} = 4.5 ft/d



LNAPL Saturation at 1.3 days

1,161,000 gallons
Kx / Kz = 100
Dip: 3% (1.7 degrees)
Time = 4.3 Days



LNAPL Saturation at 4.3 days

Key Points:

- **Continuous release of 270,000 gpd reaches water table in 1.3 days**
- **LNAPL travels along the water table 200 ft to the east and 700 ft to the west by 4.3 days (in 3 more days).**
- **Simple LNAPL model estimates are conservative, as it does not consider displacement of water, which would reduce migration**

What catastrophic continuous release of LNAPL reaches the water table and when?

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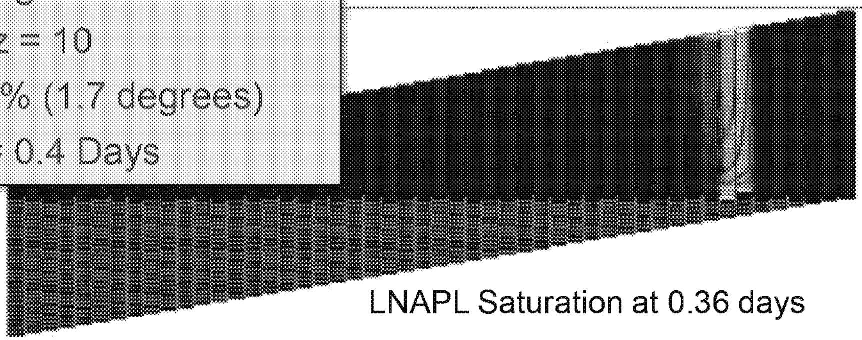
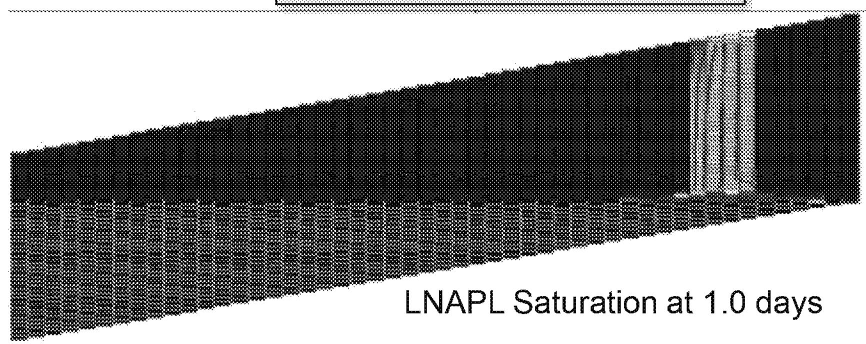
97,000 gallons
Kx / Kz = 10
Dip: 3% (1.7 degrees)
Time = 0.4 Days



LNAPL Saturation at 0.36 days

Test Model 2: K_{wz} = 45 ft/d

270,000 gallons
Kx / Kz = 10
Dip: 3% (1.7 degrees)
Time = 0.4 Days



LNAPL Saturation at 1.0 days

Key Points:

- **Continuous release of 270,000 gpd – LNAPL reaches water table in 0.36 days**
- **LNAPL travels along the water table 200 ft to the east and 200 ft to the west by 1.0 days (in 0.64 more days).**

What large continuous release of LNAPL reaches the water table and when?

- With continuous release of 270,000 gpd, LNAPL reaches water table in 0.36 to 1.3 days
- Migration along water table of about 200 feet occurs in 0.64 to 3 days

- ***The simulations are a test case to demonstrate the proposed approach. The domain will be expanded to include all locations of concern, and the LNAPL modeling objectives will be implemented for the actual evaluations***

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Potential Path Forward

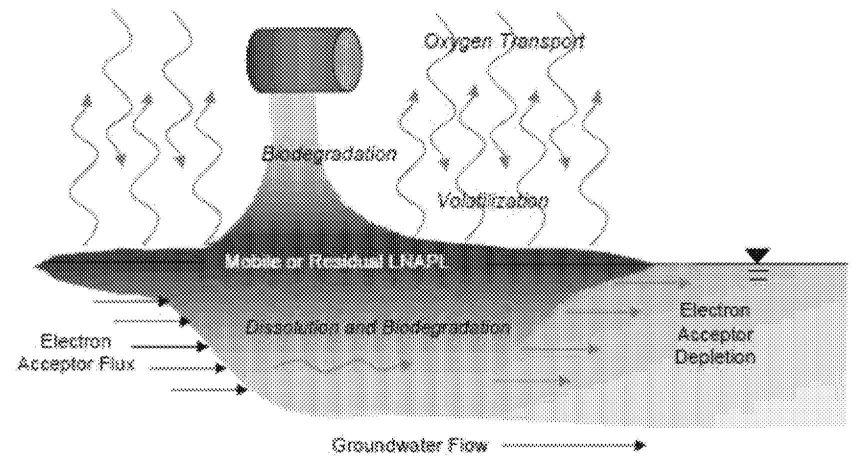
Potential Path Forward

- Gain alignment on a reasonable range of values for key parameters and calibration metrics (March 2019 Face-to-Face Meetings)
- Initial model test runs can help to inform key issues related to LNAPL simulation at Red Hill, and could be used to further develop the Red Hill LNAPL modeling effort
- Revise test model domain extent to include key features that may impact LNAPL flow
  - Cover full extent of all tanks with sufficient uphill coverage to NE
  - Past Red Hill Shaft to SW
  - Include Moanalua Valley as a boundary to SE
  - Include Halawa Shaft and slightly beyond to NW
  - Conceptually include partial barriers below N and S Halawa Valleys above water table
    - Two cases if needed, to evaluate impact of longer versus shorter barrier
- Revise grid to have finer representation near tanks as needed
- Develop models to meet LNAPL modeling objectives
- Calibrate models to bound information available on known historical spills

Potential Path Forward

- Apply models to evaluate holding capacity model
- Apply models to understand impact of various uncertainties
- Apply models appropriately for various scenarios of interest, per the LNAPL modeling objectives

Potential Application Scenarios



- Release cases
  - Low Release
  - Intermediate Release (2014)
  - Large
  - Catastrophic Release
- Release locations
  - At tank which is most downhill
  - At tank which is most uphill
  - Release from Lower Access Tunnel
- Saprolite barrier cases
  - Longer barrier indicating deeper saprolite outcropping later
  - Shorter barrier indicating shallower saprolite outcropping earlier
- Stacked release scenarios
  - Include decay rate for residual LNAPL